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Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

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Agency Code:

Proposal Number: 73638CHCF   **Agreement Number: W911NF-18-1-0430**
INVESTIGATOR(S):

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Report Date: 15-Feb-2019   Date Received: 23-Jan-2019
Final Report for Period Beginning 16-Aug-2018 and Ending 15-Feb-2019
Title: 26th Current Trends in Computational Chemistry
Begin Performance Period: 16-Aug-2018   **End Performance Period:** 15-Feb-2019
Report Term: 0-Other
Submitted By: Jerzy Leszczynski   Email: jerzy@icnanotox.org
                                     Phone: (601) 979-3723
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 0   **STEM Participants:** 24

Major Goals: The major goals of this project are to 1) provide a platform for discussing applications and the latest developments of computational chemical techniques and to 2) provide graduate and undergraduate students with an opportunity to present their research work at an international meeting.

Accomplishments: This year, the ICN, in partnership with Jackson State University and the US Army Corps of Engineers, hosted the 26th International Conference on Current Trends in Computational Chemistry and hosted over 130 participants from 8 countries.
    The format of the 26th CCTCC consisted of 6 sessions of (invited) plenary lectures and over 60 poster presentations covering applications as well as theory. Over 40 of the poster presentations were given by graduate and undergraduate students. A total of 9 prizes ranging from first place to honorable mention were awarded for the best undergraduate and graduate poster presentations.
    The 26th CCTCC included lectures and seminars from noted scientists in the profession.
    The supporting agencies were the Army Research Office (ARO), National Science Foundation (CREST and EPSCoR Programs); Office of Naval Research; Parallel Quantum Solutions; Springer; and US Army Corps of Engineers.
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Training Opportunities: Graduate, undergraduate, and high school students participated in two poster sessions highlighting student results from research activity.

Over 40 of the poster presentations were given by graduate and undergraduate students. A total of 9 prizes ranging from first place to honorable mention were awarded for the best undergraduate and graduate poster presentations.

Results Dissemination: The 26th Current Trends in Computational Chemistry Conference proceeding was disseminated during the CCTCC.

The full document is provided in the "upload" section.

Honors and Awards: Graduates and undergraduates received a total of 9 prizes ranging from first place to honorable mention for the best undergraduate and graduate poster presentations.

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Jerzy Leszczynski
Person Months Worked: 1.00   **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Other (specify)
Participant: Shonda Allen
Person Months Worked: 1.00   **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Other (specify)
Participant: Galina Lobodina
Person Months Worked: 1.00   **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

International Conference on Current Trends in Computational Chemistry
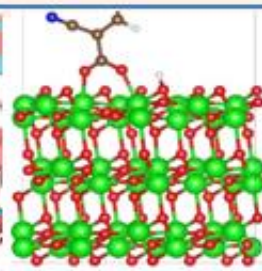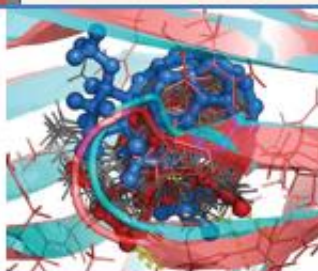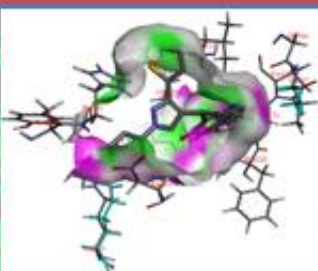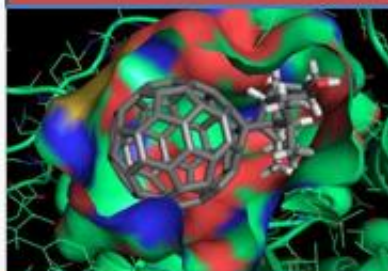
2018

CCTCC

November 9−10, 2018
Jackson, MS

JSU | JACKSON STATE UNIVERSITY

INTERDISCIPLINARY CENTER for NANOTOXICITY

Springer

US Army Corps of Engineers

National Science Foundation

Organizing Committee

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Delbert Bagwell	U.S. Army Corps of Engineers
Jaroslav Burda	Charles University in Prague
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Galina Lobodina	Jackson State University

Support

Army Research Office

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National Science Foundation (EPSCoR Program)

Office of Naval Research

Parallel Quantum Solutions

Springer

US Army Corps of Engineers

Friday, November 9, 2018

8:00A – 12:00P	Registration	
8:00A – 9:00A	Coffee and morning snacks	
9:00A - 9:10A	Opening Remarks	
9:10A - 10:40A	**1st Session** **Session Chair: P. Pulay**	**Prof. Henry F. Schaefer** "Quantum Chemistry and Large Scale Computations: A Tightly Coupled Parallel Development" **Richard Wong Ming Wah** "Applications of Halogen Bonding to Supramolecular Chemistry, Phosphorescence Materials and Catalysis"
10:40A–11:00A	Coffee Break / Pictures	
11:00A–12:30P	**2nd Session** **Session Chair: A. Gajewicz**	**Leslie Vogt-Maranto** "Molecular dynamics via machine learning: Predicting energies from electron densities" **Masataka Nagaoka** "Red Moon Methodology: A Computational Molecular Technology for Complex Chemical Reaction Systems - Its Theoretical Treatment and Applications"
12:30P -2:00P	Lunch	
2:00P -3:30P	**3rd Session** **Session Chair: J. Murray**	**Marivi Fernández-Serra** "Evaluating photocatalytic active sites as function of polarization, level alignment and spontaneous dissociation of hydroxyl groups at perovskite oxide surfaces" **Laura Gagliardi** "Computationally Guided Discovery of Metal–Organic Frameworks Active for Catalysis"
3:30P -3:50P	Coffee Break	
3:50P – 5:30P	First Poster Session (P1)	
6:00P – 8:00P	Dinner	

Saturday, November 10, 2018

8:00A – 9:00A	Coffee and morning snacks	
8:30A – 11:00A	Registration	
9:00A – 10:30A	**4th Session** **Session Chair: A. Wierzbicki**	**Margarita Isabel Bernal Uruchurtu** "A tale of water and halogens and the toolbox needed to unveil their narrative" **Tomasz Puzyn** "Towards computational risk assessment of ionic liquids"
10:30A -10:50A	Coffee Break	
10:50A-12:20P	**5th Session** **Session Chair: M. Shukla**	**Katharina Boguslawski** "Inexpensive wave-function-based methods to model ground and excited states in challenging systems" **Frank Hagelberg** "Zigzag Nanoribbons as Media for Spin Transmission"
12:20P – 2:00P	Lunch	
2:00P – 4:15P	**6th Session** **Session Chair: A. Sygula**	**YounJoon Jung** "Computer Simulation Study of Differential Capacitance and Charging Mechanism in Ionic Liquid-Based Graphene Supercapacitors" **Jozef Adam Liwo** "Physics-based scale- and geometry-consistent coarse-grained potentials" **Joachim Sauer** "Ab initio calculations with chemical accuracy for molecule - surface interactions and the performance of DFT+dispersion"
4:15P- 4:40P	Coffee Break	
4:40P- 6:00P	**2nd Poster Session** (P2)	
6:30P – 9:00P	Banquet	Banquet Speaker **David Horner**, Director of ERDC ITL

Invited Speakers

1st Session

Henry F. Schaefer

"Quantum Chemistry and Large-Scale Computations: A Tightly Coupled Parallel Development"
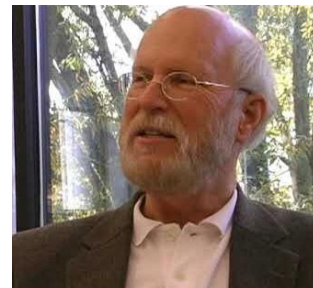
Richard Wong Ming Wah

"Applications of Halogen Bonding to Supramolecular Chemistry, Phosphorescence Materials and Catalysis"

2nd Session

Leslie Vogt-Maranto

"Molecular dynamics via machine learning: Predicting energies from electron densities"

Masataka Nagaoka

"Red Moon Methodology: A Computational Molecular Technology for Complex Chemical Reaction Systems - Its Theoretical Treatment and Applications

3rd Session

Marivi Fernández-Serra

"Evaluating photocatalytic active sites as function of polarization, level alignment and spontaneous dissociation of hydroxyl groups at perovskite oxide surfaces"

Laura Gagliardi

"Computationally Guided Discovery of Metal–Organic Frameworks Active for Catalysis"

4th Session

Margarita Isabel Bernal Uruchurtu

"A tale of water and halogens and the toolbox needed to unveil their narrative"

Tomasz Puzyn

"Towards computational risk assessment of ionic liquids"

5th Session

Katharina Boguslawski

"Inexpensive wave-function-based methods to model ground and excited states in challenging systems"

Frank Hagelberg

"Zigzag Nanoribbons as Media for Spin Transmission"

6th Session

YounJoon Jung

"Computer Simulation Study of Differential Capacitance and Charging Mechanism in Ionic Liquid-Based Graphene Supercapacitors"

Jozef Adam Liwo

"Physics-based scale- and geometry-consistent coarse-grained potentials"

Joachim Sauer

"Ab initio calculations with chemical accuracy for molecule - surface interactions and the performance of DFT+dispersion"

Source of the photo: Humboldt-Stiftung/Peter Himsel

Banquet Speaker

David Horner
Director of ERDC ITL

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Conference on Current Trends in Computational Chemistry 2018

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Structures, Energetics, and Vibrational Frequencies of Microhydrated Hexafluorophosphate, $PF_6^-(H_2O)_{n=1,2}$, from DFT and Ab Initio Computations

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This study systematically examines an anion commonly used in room temperature ionic liquids, hexafluorophosphate (PF_6^-), and its noncovalent interactions with up to two explicit water molecules ($PF_6^-(H_2O)_n$, where n = 1, 2). Initial low energy configurations were identified via a set of relaxed angular scans across the edges and faces of the PF_6^- octahedron using the global hybrid M06-2X density functional with a triple-ζ correlation consistent basis set augmented with diffuse functions on all non-hydrogen atoms (cc-pVTZ for H and aug-cc-pVTZ for P, O, F; denoted haTZ). Full geometry optimizations were performed on these initial structures using a variety of common density functionals theory (DFT) methods (B3LYP, B3LYP-D3, M06-2X, and ωB97XD) as well as the MP2 *ab initio* method with the same haTZ basis set. The corresponding harmonic vibrational frequencies were computed for every stationary point identified. Analogous CCSD(T)/haTZ computations are underway in order to gain additional insight on the $PF_6^-(H_2O)$ and $PF_6^-(H_2O)_2$ potential energy surfaces while also serving as a comparative benchmark for the DFT and MP2 results. A new $PF_6^-(H_2O)_2$ minimum has been identified that is approximately 2 kcal mol^{-1} lower in energy than any other structure previously reported in the literature [1,2]. For the $PF_6^-(H_2O)_1$ system, DFT computations identify two unique stationary points competing for the lowest energy configuration, which is consistent with prior work [1]. However, only one of these structures is a stationary point on the MP2 potential energy surface. This result suggests that some DFT methods might not correctly describe the interaction between PF_6^- and H_2O.

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Systematic Approach to Understanding Molecular Reorganization and Mechanism in Biochar

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Biochar is an important by-product of the pyrolysis of biomass. Biochar is important because of its application in soil amendment, carbon sequestration, and absorbance of pollutants in our environment. In this study, we aim to understand the molecular reorganization and mechanism in biochar. By examining the thermal decomposition of glucose we aim to understand similar mechanisms in biochar. Examining fragmentation of glucose and taking a look at bond energy between each bond formed in glucose we see the most stable conformation of the fragments formed.

Density Functional Theory Analysis of Nitro-Polycyclic Radical Derivative from UV-Vis Excitation

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Polycyclic aromatic hydrocarbons (PAHs) are a large group of organic compounds that are comprised of two or more merged benzene rings arranged in various configurations. These molecules are generated from the incomplete combustion of organic materials such as burning of wood, coal, oil. PAHs have physicochemical properties that make them highly mobile in the environment such as high melting and boiling points, low vapor pressure, and very low solubility in aqueous solutions. These listed properties allow them to be omnipresent which creates a health issue for all life.

Nitrated polycyclic aromatic hydrocarbons (NPAHs) are omnipresent on earth are considered atmospheric pollutants. These molecules are of prime concern because many of them are more carcinogenic than their parent PAHs. Although NPAHs aren't as potent as their parent molecule, they possess a greater degree of mutagenicity. The NPAH of this study is 3-Nitrofluoranthene (3-NFA) and how after UV excitation it produces a carboxyclic acid derivate. Photoreaction kinetics of NPAHs has a variety of possible reaction pathways to yield the final product. A potential degradation pathway was constructed. To asses this outcome this potential degradation pathway all the components will be calculated using Time-Dependent Density Functional Theory (TDDFT) calculations. In this experiment a NPAH radical is examined through UV-Vis excitation and H-NMR. Implementing the functional CAM-B3LYP with basis set 6-311++G(d) to produce a theoretical standard to compare the experimental data to assist in conforming the predicted degradation scheme.

Computational Exploration of Double Nitrogen Doping of 1,2-, 1,3- and 1,4-Substitutions in Multiple Rings of Graphene

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Nitrogen-doped graphene has been of recent interest to manipulate the properties of graphene. Many studies revealed that heteroatom doping with graphene is one of the efficient approaches for tuning its electronic and chemical properties. In this study, we considered the finite-sized graphene model, $C_{186}H_{36}$ to investigate the double nitrogen doping within six-membered rings of the graphene. Three possibilities of dinitrogen doping are 1,2-, 1,3- and 1,4-substitutions. Our systematic study presents the results of positional preference of double nitrogen doping involving multiple non-equivalent six-membered rings. Our aim is to investigate the positional preference of three different doping possibilities and the selectivity of rings for doping of two nitrogen atoms. All structures were optimized using density functional theory (DFT) B3LYP/6-31G(d) level. HOMO-LUMO energy gap values for all the positional isomers were calculated using TPSSh/6-31G(d)//B3LYP/6-31G(d) level. All the calculations were performed using Gaussian 16 program package. The relative stabilities of these isomers are found to follow the trend in majority of six-membered rings: 1,4- > 1,3- > 1,2-substitution. Interestingly, the stabilities of double nitrogen dopants in all three types of substitutions depend on the doping location. Our computational study predicts that the most stable isomers have two nitrogen atoms doped close to the zigzag edge. However, the nitrogen doping at the armchair edge provides the structures with high relative energies. We have analyzed the effect of nitrogen dopants in graphene on HOMO and LUMO energies and HOMO-LUMO energy gaps.
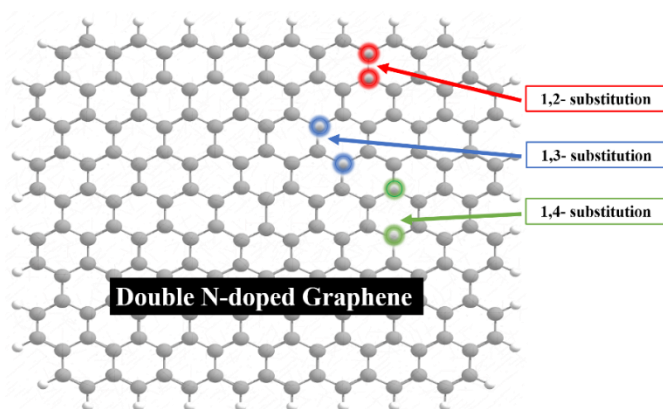
The Influence of N-Aryl-Naphthylamine Derivatives' Conformations on LEDGF/P75-IN PPI Inhibition

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Design of effective drugs is one of the most substantial goals of computational chemistry nowadays. None of the existed medication can fully treat the dangerous venereal disease AIDS. However, various drugs that could inhibit HIV activity have been discovered and studied. "LEDGINs" are the small compounds that inhibit LEDGF/p75-IN PPI. They have proven a good antiviral activity. Some of the representatives of this class of inhibitors are N-aryl-naphthylamines. Crucitti et al. [1] have analyzed the inhibitory activity of various N-aryl-naphthylamines towards HIV. The idea, that a carboxylate functional group has a positive influence on the inhibition activity has been proposed, hoverer not completely proven. Some compounds having the carboxylic and methyl-carboxylic groups have also shown low or no activity at all.

In order to perform more comprehensive study our idea was to discover the influence of existent conformations of each compound on an inhibition process. In N-aryl-naphthylamines molecules the free rotation of naphtyl and phenyl rings occurs. Hindered rotation of big fragments, steric perturbations and other factors can cause the existence of several stable conformations for such compounds. Since all the stable conformations have their lifetime, each of them has their own impact, playing a critical role in inhibition processes. In order to explain this, we have performed the conformational study of 37 compounds. Experimental data of alphascreen % inhibition for these compounds test has been published in [1].

Relaxed scan calculations have been performed at the B3LYP/3-21G level of theory using Gaussian 09 with CPCM model in water solvent. The surface of studied compounds has shown to be uneven with four or more local minima. In most cases all four minima being different in geometrical structure has the same or similar populations. Minima obtained from surface scan have been calibrated by optimization at B3LYP/6-31G_ESKJ level of theory. Populations of conformers have been calculated using Boltzmann distribution method for further quantitative structure-activity relationship (QSAR) and docking study. We have performed the molecular docking in order to clarify whether conformational effect has any influence on a ligand docking. Obtained results have demonstrated desirability of conformational analysis prior to molecular docking studies.

[1]   G. Cuzzucoli Crucitti, L. Pescatori, A. Messore, V.N. Madia, G. Pupo, F. Saccoliti, L. Scipione, S. Tortorella, F.S. Di Leva, S. Cosconati, E. Novellino, Z. Debyser, F. Christ, R. Costi, R. Di Santo, Discovery of N-aryl-naphthylamines as in vitro inhibitors of the interaction between HIV integrase and the cofactor LEDGF/p75, Eur. J. Med. Chem. 101 (2015) 288–294. doi:https://doi.org/10.1016/j.ejmech.2015.06.036.

Conformational Energetics of Urea and Thiourea
Near the CCSD(T) Complete Basis Set Limit

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This study provides the first relative conformational energies near the CCSD(T) complete basis set limit for the low-lying stationary points of urea and thiourea. Full geometry optimizations were performed on ten conformations of urea and eight conformations of thiourea using the MP2 method and a series of Dunning's correlation consistent basis sets (cc-pVXZ where X = D, T, Q, and 5; denoted XZ). Harmonic vibrational frequencies were computed to characterize each stationary point as a minimum ($n_i = 0$), transition state ($n_i = 1$) or higher order saddle point ($n_i \geq 2$) on each potential energy surface. Additional computations were performed with an extra set of tight "d" functions placed on sulfur (using cc-pV(T+d)Z for S and cc-pVTZ for C, H, and O) and were found to have no impact on the relative energies. Five urea conformations and four thiourea conformations with relative energies lower than 10 kcal mol^{-1} were then optimized at the CCSD(T)/TZ level of theory. Single-point energy computations were then performed upon the CCSD(T)/TZ optimized geometries at the CCSD(T)/XZ level of theory, where X = D, T, Q, 5, and 6.

Cancer Cell Imaging and Study the Interaction of Multiple Types of Drugs By Using Red Emissive Carbon Dots

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Cancer is the second leading cause of death worldwide and was responsible for 8.8 million deaths in 2015 globally. According to the World Health Organization, nearly 1in 6 deaths is due to cancer. Cancer is a generic term for a large group of diseases that can affect any part of the body. One defining feature of cancer is the rapid growth of abnormal cells that grow beyond their usual boundaries, and which can then invade adjoining parts of the body and spread to other organs, the latter process is referred to as metastasizing. Metastases are a major cause of death from cancer. The most common cancers are lung (1.69 million deaths), Liver (788,000 deaths), colorectal (774,000 deaths), stomach (754,000 deaths) and breast cancer (571,000 deaths). Breast cancer is the most common cause of cancer death among US women. According to U. S. Breast Cancer Statistics, about 1 in 8 U.S. women (about 12%) will develop invasive breast cancer over the course of her lifetime. In 2017, there was an estimated 252,710 new cases of invasive breast cancer, 63,410 new cases of breast carcinoma in situ, and 40,610 breast cancer deaths. Therefore, it is important to detect breast cancer at an early stage to increase the chances for successful treatment. Recently, carbon-based fluorescent nanomaterials, such as carbon dots (CDs), have attracted much attention because of their unique optical properties and their low to non toxic features. Alternatively, this new class of nanomaterials is considered to be a potential substitute to semiconductor Quantum Dots (QDs). The aim of this study was to detect the cancer cells and image them with red emissive carbon dots, synthesized from 1, 4-phenylenediamine. We picked this organic dye because this is cost effective and easy to handle. Moreover, in this experiment we have studied the binding mechanism of different drugs such as neurotransmitters and anticancer etc., to find the multiple interactions and selectivity using the fluorescence technique. We also used several spectroscopic and imaging techniques such as UV-vis, Fluorescence, FTIR, TEM, for characterization and studied the compositions of these compounds and used them for cell imaging of breast cancer cells SK-BR-3.

Keywords: Red emissive carbon dots, SK-BR-3, UV-vis, Fluorescence, TEM, FTIR

# Theoretical investigation on the degradation mechanism of the insecticide formetanate with OH radicals

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Formetanate (FMT) is an acaricide and insecticide widely used in agriculture. FMT possesses two functional groups, a carbamate group and a formamidine group (See Fig. 1), both acting as competitive inhibitors of important neurotransmitters [1]. Due to its high toxicity and high solubility in water, FMT a potential hazard to human and animal health. Thanks to the development of advanced oxidation processes (AOPs), such as Fenton reaction, photo-Fenton, H_2O_2/UV, etc., it is now possible to partially or totally remove contaminants from water [2]. For instance, Alberto and Jagannathan along with their co-workers [3,4], reported AOPs in which OH radicals ($\cdot$OH) were generated to degrade FMT. In these works, authors used MS techniques to monitor the degradation products. However, to explain the *m/z* signals obtained, none of the authors suggested the addition of $\cdot$OH to the formamidine group. Instead, they suggested that $\cdot$OH is added to the aromatic ring or abstracts H atoms from the chain. In this work, based on theoretical calculations, we proposed that $\cdot$OH add primarily or at least in a competitive way to the double bond of the formamidine group. The intermediates that could be generated based on our proposal were in complete agreement with the *m/z* signals reported by the authors. All calculations were carried out with the Gaussian 09 suite of programs [5] using the PBE0/6-31++G(d,p) level of theory. Our results indicated the reaction enthalpy for addition of $\cdot$OH on the formamidine double bond to have the most negative value, followed by addition on the aromatic ring. Besides, addition of $\cdot$OH at the double bond of the formamidine group had the smallest reaction energy barrier. We also measured the charge-transfer interaction of $\cdot$OH with FMT in the transition structures (TSs) using Natural Bond Orbitals (NBO) [6] and found the TS for addition on the formamidine double bond to be the strongest. All these results pointed in one direction: the double bond of the formamidine group is the more reactive site of FMT toward $\cdot$OH. Therefore, it must be taken into consideration when trying to explain degradation products of FMT in presence of $\cdot$OH.
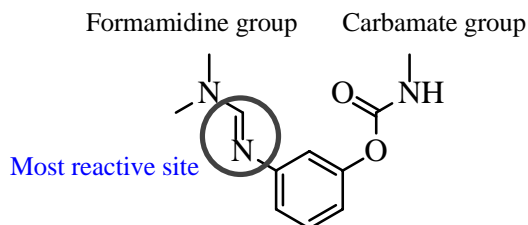
Fig. 1 Chemical structure of FMT

Inexpensive Wave-Function-Based Methods to Model Ground and Excited States in Challenging Systems

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The correlation energy is a central quantity in quantum chemistry. It is usually defined as the error in the electronic energy calculated within the independent-particle model of Hartree-Fock theory with respect to the exact solution of the electronic Schrödinger equation. Although there exists no rigorous distinction between different types of electron correlation effects, the correlation energy is typically divided into two categories: static/nondynamic and dynamic. While dynamic electron correlation effects can be accurately described by standard, well-established methods, like Møller-Plesset perturbation theory or single-reference coupled cluster theory, present-day quantum chemistry lacks simple, robust, and efficient algorithms for a qualitatively correct description of strongly-correlated many-body problems.

We present a conceptually different approach that is well suited for strongly correlated electrons, but does not use the orbital model. Our method exploits the feature that electron correlation effects can be built into the many-electron wave function using two-electron functions, also called geminals. One of the simplest practical geminal approaches is the antisymmetric product of 1-reference-orbital geminals (AP1roG) [1-4], which is equivalent to the pair-Coupled-Cluster Doubles model [3].

In this work, we discuss the performance of AP1roG-based methods [3-5] in modeling electronic structures for molecules containing light and heavy elements, including actinides. We will present different excited state models [6-8] that allow us to target singly- and doubly-excited states with electron-pair theories. Our study indicates that geminal-based approaches provide a cheap, robust, and accurate alternative for the description of electron correlation effects in both ground and excited states.

How Can Steric Hindrance Be Alleviated in the Formation of Dendrimer Precursors to Conserve π-Conjugation?

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The Mississippi College Organic Research Group (MC-ORG) has an ongoing mission to design and prepare flat, two-dimensional dendrimers. In order for dendrimers to attain light-harvesting properties, conjugation of the π-bonding system must be conserved. It has been found that when twisting occurs about the single bonds of the dendrons, there is a decrease in energy transfer and therefore loss of conjugation and reduced light harvesting properties. In previous projects, the MC-ORG has been synthesizing dendrimers that show twisting, and therefore loss of π-conjugation, due to the hydrogens in the ortho positions of the phenyl rings. In order to alleviate these steric interactions, the MC-ORG group is attempting to synthesize structures that incorporate diynes. The hope is that the extended length of the diyne units, as opposed to the ethynyl units previously used, will position the hydrogens far enough from one another that their steric interactions will be reduced and twisting of the structure will not occur. The goal of this project is to assist the MC-ORG in determining whether these structures will alleviate the twisting and produce "flat" dendrimers that retain conjugation. Another goal of this research is to determine if twisting can be eradicated by changing the types of atoms and the length of the bridges that connect the phenyl rings. Eventually, NICS calculations will also be conducted to determine the aromaticity of the structures and prove whether conjugation is truly conserved. To investigate these questions, optimum structures are computed at the SCF and DFT levels of theory. The functionals employed are B3LYP, M06-2X, and ωB97XD. All calculations use correlation consistent basis sets. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Regioselectivity of Acid-Catalyzed Epoxide Ring-Opening Reactions

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Epoxide opening reactions occur through two known mechanisms: base catalyzed, in which nucleophilic attack opens the ring, followed by a proton transfer to produce the substituted alcohol, and acid catalyzed, in which the oxirane oxygen is protonated via proton transfer, followed by nucleophilic attack to produce the substituted alcohol. There is little debate in the literature about base catalyzed reactions involving the least substituted carbon in the epoxide due to the lack to steric hindrance to nucleophilic attack, presumably since the mechanism of such attack is S_N2. Two leading undergraduate textbook authors, however, disagree about the regioselectivity involving acid catalyzed epoxide opening reaction when the carbons are primary and secondary. Joel Karty asserts that the more substituted carbon is attacked in the acid catalyzed mechanism and offers bond length data to augment his argument. David Klein, on the other hand, suggests that the less substituted carbon is attacked when the competing electrophiles are primary versus secondary due to "the steric effect predominating over the electronic effect."

To investigate these dissenting opinions, we consider a series of asymmetric derivatives of oxirane. Specifically, the optimized equilibrium geometries of 2-methyloxirane, 2,2-dimethyloxirane, 2,2,3-trimethyloxirane, 2-ethyloxirane, 2,2-diethyloxirane, 2,2,3-triethyloxirane, 2-tert-butyloxirane, and 2,2-di-tert-butyl-oxirane are computed using SCF theory, second-order perturbation theory (MP2), and density functional theory. The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ωB97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets, cc-pVDZ and cc-pVTZ. Bond lengths should be indicative of bond strength, thus the different C-O bonds are compared in each optimized structure. Then the oxygen of each system is protonated, and the geometry of each is again optimized and compared. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Noncovalent Interactions in Networks of Trimethylamine *N*-oxide, Guanidinium Cation, and Water

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Guanidinium chloride, trimethylamine *N*-oxide (TMAO), and urea all belong to a small class of organic compounds called osmolytes, which have been studied extensively because they play an important role in biological functionality. Urea and guanidinium chloride are known to denature proteins while TMAO promotes their folding. All of these systems contain many sites for hydrogen bonding, and interactions with water are certainly important to their biological functionality and their abilities to influence protein stability. In previous work, we have studied networks of TMAO, urea, and water to begin to understand how TMAO can promote folded protein stability and also counteract the denaturing effect of urea. In the current study, we have replaced urea with guanidinium cation to see if the interactions are similar or different. Optimum geometries and the corresponding vibrational frequencies of networks of TMAO, guanidinium cation, and water have been computed using density functional theory. The DFT functionals employed are the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ωB97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are two of Dunning and coworkers' correlation consistent basis sets with diffuse functions: aug-cc-pVDZ and aug-cc-pVTZ. In addition, implicit solvation effects have been examined using the polarizable continuum model for solvation with water as the solvent on many of the optimized networks identified. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Conventional Strain Energies of Cyclopropane, Aziridine, Oxirane, Silirane, Phosphirane, and Thiirane

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The conventional strain energies for cyclopropane, aziridine (Figure 1), oxirane (Figure 2), silirane (Figure 3), phosphirane (Figure 4), and thiirane (Figure 5) are determined within the isodesmic, homodesmotic, and hyperhomodesmotic models to compare the effect of third-row elements to second-row elements on the strain energies of three-membered rings. Optimum equilibrium geometries, harmonic vibrational frequencies, and corresponding electronic energies are computed for all pertinent molecular systems using self-consistent field (SCF) theory, second-order perturbation theory (MP2), and density functional theory (DFT). The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional and the M06-2X high nonlocality hybrid functional from Thular and Zhao. The basis sets employed are Dunning and coworkers' correlation consistent basis sets: cc-pVDZ, cc-pVTZ, and cc-pVQZ. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.
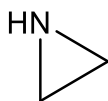

Figure 1. Aziridine
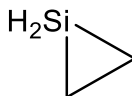

Figure 2. Oxirane

Figure 3. Silirane

Figure 4. Phosphirane

Figure 5. Thiirane

DFT Study on Binding of Histidine and Proline with Graphene in Gas and Aqueous Phases

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Quantum chemical calculations using M06-2X/6-31G(d) level have been performed to understand the interactions between two α-amino acids (histidine and proline) individually with graphene. Two finite size graphene sheets containing 62 and 183 carbon atoms were considered and their edges were terminated with hydrogen atoms. For each of the two amino acids, we have performed the conformational analysis using MMFF force field implemented in Spartan '16. From the conformers, we have chosen 3-4 most stable and 1-2 least stable conformers for proline and histidine to build the complexes with graphene. In case of forming the complexes, we have taken into account different possible orientations. The complexes were fully optimized at the M06-2X/6-31G(d) level using Gaussian 16 program package. Binding energies with and without basis set superposition error (BSSE) were calculated. The solvation effect on binding energies was evaluated by polarizable continuum model (PCM). HOMO-LUMO energy gaps were calculated at the TPSSh/6-31G(d)//M06-2X/6-31G(d) level. Our aim is to understand the binding affinity of histidine and proline with graphene in the gas and aqueous phases, and the effect of varying the graphene sheet on the binding affinity. In case of histidine-graphene complexes, the competition between π–π and C-H/N-H⋯π interactions exists. It should be noted that histidine exhibits higher binding energy than proline. This could be attributed to the presence of π-electrons and two nitrogen atoms in the five-membered ring of histidine. The most stable complex of proline-graphene shows multiple C-H⋯π interactions along with N-H⋯π interactions. Graphene size effect is negligible for both amino acids. Inclusion of solvent (water) reduces the binding energy slightly but the trend is retained. The binding energy is generally decreased in aqueous phase. Binding of proline and histidine does not change the band gap of graphene.

Computational Study on Binding of Selected Metal Ions with Phenylalanine Dipeptide

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Systematic conformational analysis was performed on the homo-dipeptide of aromatic α-amino acid phenylalanine using MMFF force field implemented in Spartan '16 program. First twenty most stable dissimilar structures out of 492 conformers were selected for optimizations at the HF/3-21G and M06-2X/6-31G(d) levels. In the next step, three lowest energy conformers and one high energy conformer were selected from the list of twenty optimized structures to examine metal ion (Na^+, K^+, Mg^{2+} and Ca^{2+}) binding with those three conformers. Different binding modes were considered for each of the conformer with each of the metal ion. Therefore, several complexes were examined. All the complexes were fully optimized using M06-2X/6-311+G(2d,2p) level followed by frequency calculations in order to confirm whether the complexes are minima or not. The binding energies with and without BSSE correction were obtained. Expectedly, Na^+ binds stronger than K^+, and Mg^{2+} binds stronger than Ca^{2+} with phenylalanine dipeptide. The four conformers considered here exhibit the binding energy range of 26-52 kcal/mol for Na^+, 18-41 kcal/mol for K^+, 140-257 kcal/mol for Mg^{2+}, and 94-190 kcal/mol for Ca^{2+}. The binding energy values show high range for all the metal ions. It should be noted that multiple weak nonbonding interactions such as cation-π, lone pair-cation, C-H…π play vital role in determining the strength of metal ion-dipeptide binding. Our study reveals that metal ion binding with two aromatic rings and also with lone pair electrons of oxygen produces significantly high binding energy values. The high energy conformer (**2P4**) produces the most stable complex for Na^+, K^+ and Ca^{2+} metal ions.

Correlational Study between Ionic Influence and Acetylcholine Ion's Ability to Bind with DNA

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Deoxyribonucleic acid, otherwise referred to as DNA, is a composite biological molecule that resides within all living organisms. The structure of DNA is comprised of nucleotides that contains three subunits: a deoxyribose sugar, a phosphate and one of the four following organic bases- adenine (A), thymine (T), cytosine (C), and guanine (G). The organic bases have classifications as either purines or pyrimidine, with adenine and thymine being purines and cytosine and guanine being pyrimidines. The purines, which represent organic aromatic compounds, have a specific job to attach only to pyrimidines, which is known for its six-membered pyrimidine ring. Adenine, as it is paired with thymine, is inclusive of only two hydrogen bonds. On the other hand, as cytosine is to guanine, there are the three hydrogen bonds. The third bond, which enables a stronger bond to be made, occurs in the exocyclic amino acid group for guanine and in the C2 keto group for cytosine. Reviewing the entirety of DNA, it is majorly covered by phosphate backbone which acts as protection for the bases that are on the inside. Taking into consideration that the backbone only covers most of the bases inside, every molecule of DNA has major and minor grooves. Hydrogen bonds enable proteins to bind to the floor of the grooves. The hydrogen bonds act as a main component in assisting the production and function of the bases of DNA and base pairing.

Acetylcholine, a compound which occurs throughout the nervous system, functions as a neurotransmitter. Acting as the chief of the parasympathetic nervous system, which is part of the autonomic nervous system and a branch of peripheral nervous system, acetylcholine is synthesized in neurons by choline Acetyltransferase. In a study entitled: Choline Ion Interactions with DNA Atoms Explain Unique Stabilization of A-T Base Pairs in DNA Duplexes. Findings yielded that the A-T base became stronger than C-G base, which basically defies the law of the C-G being the more stable pair. Having a microscopic viewpoint revealed that choline ions bound through multiple hydrogen bonding networks with DNA atoms stably, versus the sodium ion that bound closely rather than stably. The affinity of choline ion for the minor groove of A–T base pairs is more than 2 times that for other groove areas. In the narrow A–T minor groove, choline ion has high affinity for the ribose atoms of thymine. Choline ions destabilize the formation of hydrogen bonds between G–C base pairs by binding to base atoms preferentially for both of duplex and single-strand DNA, which are associated with the bonds between G–C base pairs. It is from this found knowledge that DNA stability will become easier to manipulate through DNA nanodevices. It is believed that it will in turn yield new insight about the stability of DNA duplexes under crowding conditions in living cells. In coming up with new findings in the researcher's endeavors et al., the object is to utilize Molecular Dynamics for Calculations, regarding the whole strand or breaking it down and calculating both the A-T base pairing and C-G base pairing. The question

that stands is whether or not the ions (K+, Ca2+) that are being put in place have a greater impact on the DNA than the original ions observed (Na+, Mg2+).

An Ab Initio Study of Selected Heavy Metals and Biochemical Molecules as Potential Chelation Therapy

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Frequently, we are plagued with the major environmental issue of heavy metal contamination. It is of utmost importance for this to be addressed. Even more dire is that these heavy metals from the environment progress through the ecosystem until they, eventually, enter the human body. These metals lie dormant until there is an overwhelming concentration present, thus, causing heavy metal poisoning, which leads to numerous health challenges. Because of this threat to human health, it is pertinent to examine ways to rid the body of these heavy metals upon initial contamination to prevent accumulation. To investigate the proper disposal of these toxins, heavy metal ions such as Fe^{+2}, Cu^{+2}, Mn^{+2}, Co^{+2}, and Cr^{+2} are bound to histidine, which is an essential amino acid found in the body. Free energy of hydration is presented, as well as, initial studies on metal interactions with histidine. The chemical properties of these complexes will be evaluated. Furthermore, this will suggest how histidine and other biochemical molecules can be remediated. Hopefully, the results will yield a more effective means of preventing heavy metal accumulation and poisoning.
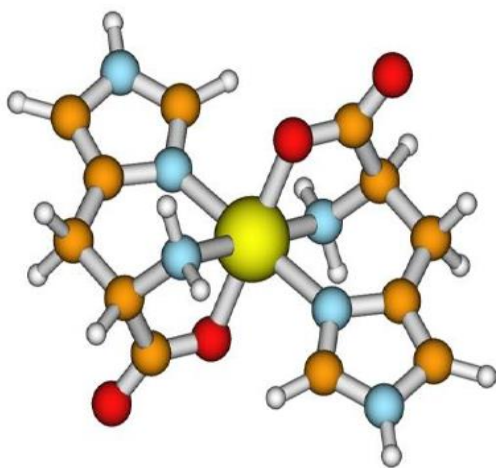
Computationally Guided Discovery of Metal–Organic Frameworks Active for Catalysis

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Metal-organic frameworks (MOFs) are attracting the attention of many scientists because of their high selectivity in gas separations, catalytic activity, and magnetic properties. We have combined theory and experiment to understand the activity of nickel and cobalt catalysts supported on Zr_6 nodes in metal–organic frameworks (MOFs) for reactions related to natural gas conversion from gas to liquid. In this lecture I will describe the methods employed to model these materials and the challenges that one faces and possible ways to advance the field.
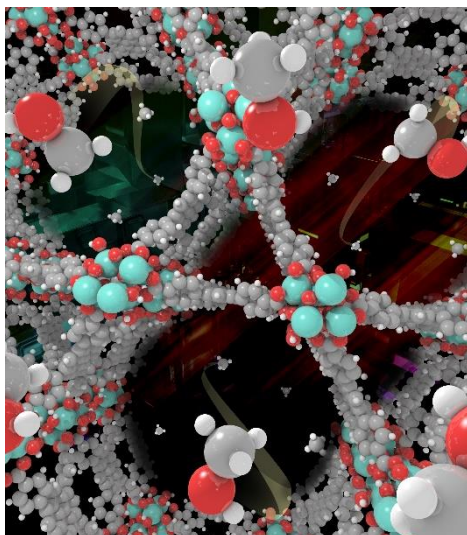
How to judge whether QSAR/read-across predictions can be trusted? Novel approach for establishing model's applicability domain

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The great need and importance of a proper and realistic assessment of the Quantitative Structure-Activity Relationship (QSAR) and read-across model's predictive power was, stressed multiple times, in the EU REACH legislation as well as in the Environmental Protection Agency (EPA), and the European Chemicals Agency (EChA) official guidance documents, which make reference to the OECD principles for QSAR validation. Among the various validation aspects addressing the uncertainty in predictions, the concept of the identification of the interpolation (true predictions) or extrapolation (less reliable predictions) region is emerged as probably one of the most important. This is because the information on the applicability domain provides evidence on reliability to enable the user of the model to judge whether the prediction for a new chemical is trustworthy and may be, therefore, accepted or not.

The intention of the present study was to propose a method for defining the interpolation space that would provide realistic assessment of the computational model's predictive ability with great attention paid to models developed from the very limited-size training sets. In the present study the new probability-oriented distance-based approach ($AD_{ProbDist}$) for determining the QSAR/read-across model's applicability domain where true and reliable predictions can be expected was proposed. By applying a traffic light analogy with green, orange and red zones, proposed method helps users assess and differentiate between acceptable and unacceptable estimates for new compounds, without any difficulty. The greatest advantage of this method and one step further beyond the currently used approaches for establishing the reliable chemical space is that the $AD_{ProbDist}$ approach is associated not only with the chemical similarity, the structural domain, and the response domain but it also addresses the confidence limits as it was stressed in OECD Guidance Document.

Computational toxicology: Read-across approach for risk assessment of industrial organic chemicals

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Over the past decade, there has been a notable rise in the use of alternative (non-animal) testing methods (i.e., computational methods) that are targeted towards the safety assessment of chemicals. Although, *in silico* methods, in particular Quantitative Structure-Activity Relationship models (QSAR) are today viewed as promising tools for screening, ranking and prioritizing of chemicals that may pose an adverse impact on humans and the environment, those computational methods still suffer from many limitations. These are mainly due to serious paucity of widely available experimental data required for the development of predictive QSAR models. In the absence of sufficient data to build an appropriately validated QSAR model one may apply quantitative read-across methods that unlike the QSAR approach, require less empirical data to perform reliable and accurate predictions used for filling data gaps.

The intention of the present work was to overcome a number of serious limitations in the popular existing *in silico* methods for filling toxicological data gaps by delivering a new quantitative read-across algorithm. In the present study a simple and transparent read-across algorithm for a pre-screening hazard assessment of industrial organic chemicals (IOCs) that heavily relies on the distance weighted k-nearest neighbor algorithm (QRA$_{k\text{-NN}}$) was introduced. The findings from this research study demonstrated that the QRA$_{k\text{-NN}}$ algorithm based on structural similarity analysis provides a simple and effective way to obtain highly accurate predictions.

Multifunctional Biochar for Highly Efficient Capture, Identification, and Removal of Toxic Metals and Superbugs from Water Samples

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According to the World Health Organization, more than two billion people in our world use drinking water sources which are not free from pathogens and heavy metal contamination. Unsafe drinking water is responsible for the death of several millions in the 21st century. To find facile and cost-effective routes for developing multifunctional materials, which has the capability to resolve many of the challenges associated with drinking water problem, here, we report the novel design of multifunctional fluorescence-magnetic biochar with the capability for highly efficient separation, identification, and removal of pathogenic superbugs and toxic metals from environmental water samples. Details of synthesis and characterization of multifunctional biochar that exhibits very good magnetic properties and emits bright blue light owing to the quantum confinement effect are reported. In our design, biochar, a carbon-rich low-cost byproduct of naturally abundant biomass, which exhibits heterogeneous surface chemistry and strong binding affinity via oxygen-containing group on the surface, has been used to capture pathogens and toxic metals. Biochar dots (BCDs) of an average of 4 nm size with very bright photoluminescence have been developed for the identification of pathogens and toxic metals. In the current design, magnetic nanoparticles have been incorporated with BCDs which allow pathogens and toxic metals to be completely removed from water after separation by an external magnetic field. Reported results show that owing to the formation of strong complex between multifunctional biochar and cobalt(II), multifunctional biochar can be used for the selective capture and removal of Co(II) from environmental samples. Experimental data demonstrate that multifunctional biochar can be used for the highly efficient removal of methicillin-resistant Staphylococcus aureus (MRSA) from environmental samples. Reported results also show that melittin, an antimicrobial peptide attached multifunctional biochar, has the capability to completely disinfect MRSA superbugs after magnetic separation. A possible mechanism for the selective separation of Co(II), as well as separation and killing of MRSA, has been discussed.

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FRET Based Theranostic Nanohybrid for Two-Photon Bioimaging and Photodynamic Therapy of Superbugs

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The need for theranostic materials that can eliminate multidrug resistant bacteria (MDRB) has called for the development of materials that can perform two photon photodynamic therapy (PDT) that can achieve a higher depth penetration in the second biological window. The need for theranostic materials that can eliminate multidrug resistant bacteria (MDRB) has called for the development of materials that can perform two photon photodynamic therapy (PDT) that can achieve a higher depth penetration in the second biological window. These materials should also be able to be used for two-photon bioimaging. We have developed gold nanoclusters (GNCs) attached graphene quantum dot (GQD) based two photon excited theranostic nanoplatform with high two-photon absorption, very strong two-photon luminescence, as well as two-photon stability in NIR region. Experimental results show strong two-photon luminescence and two photon-induced PDT, which is based on the fluorescence resonance energy transfer (FRET) mechanism, where the GQDs with very high two-photon absorption act as two-photon donors and GNCs act as acceptors. The data indicates that singlet O2 generation efficiency enhances tremendously due to the FRET process, which increases the two-photon excited PDT efficiency for multiple drug resistance bacteria. The data also shows that the nanoplatform has the capability for bright two-photon bioimaging and two-photon photodynamic therapy for MRSA and carbapenem-resistant (CRE) Escherichia coli.

Light-Induced Activation of Organo-Metallic Co-C Bond in Mecbl-Dependent Methionine Synthase- QM/MM Study

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Methylcobalamin (MeCbl)-dependent enzyme methionine synthase (MetH), plays a critical role in the catalysis of methyl group transfer from methyltetrahydrofolate (CH3-H4folate) to homocysteine. It often performs a side reaction to generate cob (II)alamin through photolysis of organometallic Co-C bond. A hybrid QM/MM method (DFT/MM and TD-DFT/MM) has been performed to explore the photochemistry of MeCbl-bound MetH. The manifold of low-lying excited states and corresponding potential energy surface (PES) of electronically excited S_1 state has been constructed as a function of axial bond lengths to elucidate the mechanism of photoinduced activation of Co-C bond inside enzyme to investigate the photolytic properties of MeCbl-bound MetH. The analysis of S_1 PES has revealed that the two different electronic states, namely metal-to-ligand charge transfer (MLCT) and the ligand field (LF), of S_1 PES are relevant to the photodissociation of Co-C bond. There are two possible pathways identified, Path A and Path B, that connect the MLCT to LF state that represent possible photodissociation mechanisms. In the case of MetH, one possible photodissociation pathway (Path B) was identified based on the energetics of MLCT and LF states. The energetically accessible Path B involves initial the detachment of Co-N_{Im} followed by a subsequent displacement of the Co-C bond prior the formation of cob(II)alamin / CH_3 radical pair (RP). The photochemical data of base-on MeCbl was compared with the computed result of MeCbl-bound MetH to understand the effect of enzymatic environment on the photolytic properties of MeCbl. On the S_1 PES the LF electronic state is higher in energy than the MLCT state for both MeCbl in solution and inside MetH, thus the MLCT region is energetically more stabilized. In compare to MeCbl in solution, the LF state is energetically higher in energy inside the enzyme which makes it easier to form RP for isolated cofactor in solution. Therefore the enzymatic environment has played a role in the destabilization of the LF state which impede the photolysis of MeCbl-bound MetH.

Relationship between size and reactivity descriptors in transition metal nanoclusters: A DFT study

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Fischer–Tropsch (FT) synthesis is a well-known method to convert syngas into valuable hydrocarbons such as gasoline, diesel, and chemicals. The chemical reactions are catalyzed more commonly by transition metals including Fe, Co and Ru. Although, only Fe and Co catalysts are commonly employed in industry because of their lower cost. Due to the various steps involved during the conversion and the variety of products that can be generated, significant variation in catalyst composition and shape affects the nature and content of the products. That is, the catalytic activity of metal nanoparticles is greatly shape and size dependent and even just an additional atom can entirely change the reactivity and stability. Also, it is possible to improve the activity and selectivity of pure catalysts by alloying them with additional metals.

All Fischer-Tropsch mechanisms known to date begin with the adsorption of carbon monoxide followed by its dissociation on a given catalyst surface. Understanding how catalyst materials modify reactivity descriptors, such as CO adsorption and dissociation energies, is key for nano-engineering materials for this type of applications.
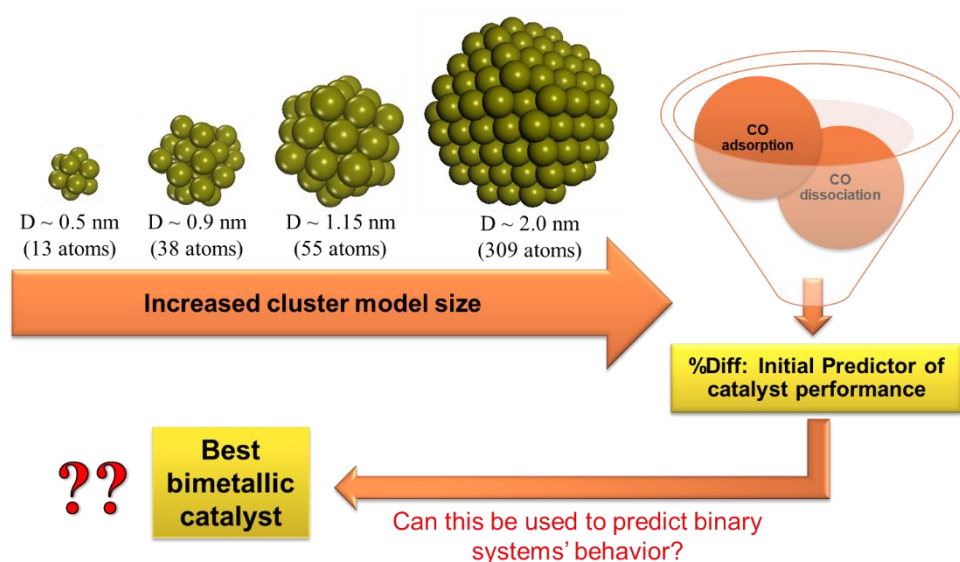

Fig.1. Selection Process of Catalyst Model

By obtaining encouraging results with our prior studies on 13-atom (~0.5 nm) cluster models of Co, Fe, Ni, Pd, Pt, and Ru, we are now investigating 55-atom (~1 nm) cluster models of the same metals using Density Functional Theory (DFT) calculations.[1] These cluster models have shown to retain the accuracy of the periodic slab models at a lower computational cost. Since experimental information at the atomic level is difficult to obtain, we carried out systematic DFT calculations for evaluating reactivity descriptors of larger models.

By applying the initial predictor [1] on 13-atom nanocluster we found that Ru has highest degree of activity to break the CO bond followed by Pd and Pt. The CO binding energy on the cluster was seen to be changed by employing core-shell structure with a different metal atom in core (alloying). For instance, by adding Pt, Pd and Ni in the core of pure Ru cluster, the CO binding energy on the cluster was seen to be increased. Cohesive energy calculation was performed for 55 atom bimetallic systems to check the stability of metal nano-cluster. Adding Ru in the core of Pt and Pd nanocluster showed improvement in cohesive energy.

These cluster-based models offer a platform for the study of the adsorption and desorption of CO and H_2 at the preliminary steps of the FT synthesis.

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Micro-and macro-hydration of (AT)$_5$ B-DNA type mini-helixes: results of density functional theory calculations

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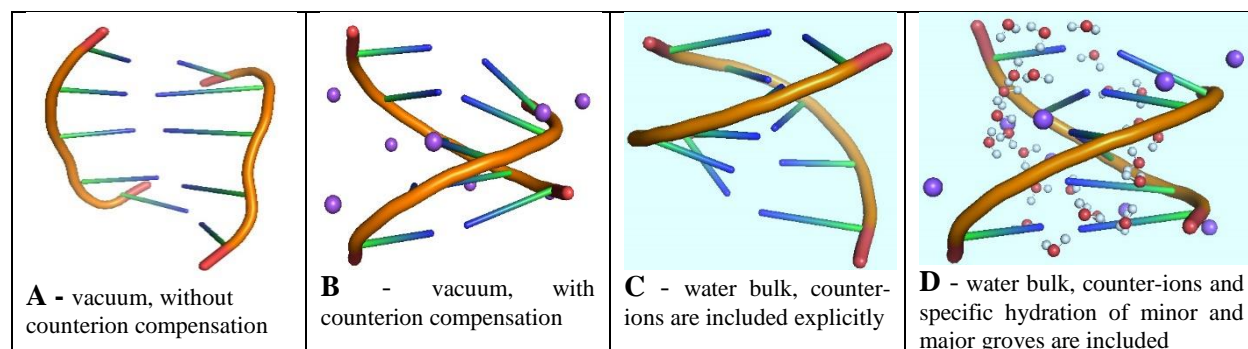
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The influence of micro- and macro-hydration on the shape of (AT)$_5$ DNA mini-helix has been studied by mean of computational modeling. The optimization of the geometry has been performed at DFT/B97-D3 level augmented by def2-SVP basis set. The presence of obtained structures to the area of local minimum has been confirmed by the validation of vibrational frequencies. The influence of water bulk has been included in the framework of CPCM model. The geometry of the key-structures is presented below (see Figure 1):

A - vacuum, without counterion compensation   **B** - vacuum, with counterion compensation   **C** - water bulk, counter-ions are included explicitly   **D** - water bulk, counter-ions and specific hydration of minor and major groves are included

Figure 1. The most important geometrical structures

Since geometrical parameters that determine a B-DNA type of structure are a slide, a roll, a twist, an inclination and an X-displacement, the evolution of those parameters as a function of the influence of surrounding is analyzed. The example of such an analysis is presented in Figure 2.
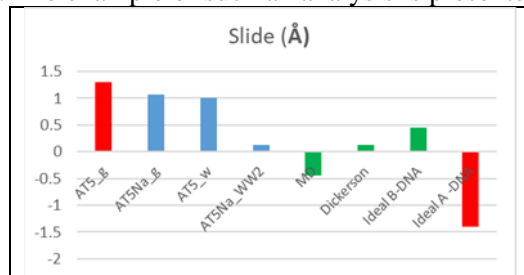
Figure 2. An evolution of Slide parameter

We concluded that the compensation of DNA helix anion by counterions is the minimal structural factor to keep it as a B-conformation. However, to obtain perfect correspondence between calculated and experimental parameters of a B-type helix (see Figure 2), the influence of all known factors (ionic atmosphere, specific hydration of minor and major grove and the influence of water bulk) have to be taken into account.

Zigzag Nanoribbons as Media for Spin Transmission

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As one of its many intriguing properties, graphene might provide an excellent medium for spin transport, and so be of high interest for applications in the field of spintronics. The respective research in experiment and theory has focused on spin injection into graphene sheets, on spin relaxation, and on ways of controlling the spin currents through graphene [1-4], to name a few areas. This presentation will highlight zigzag graphene nanoribbons (zGNRs) as active elements of spintronics and focus in particular on modified zGNR structures that might act as spin valves and spin filters. These systems are studied by density functional theory (DFT) in conjunction with Green's function analysis.

Spin-filtering devices, used to generate currents with well-defined net spin populations, are exemplified by *half metals*, materials that are metallic for one spin orientation, while acting like semiconductors or insulators for the other. Longitudinally strained zGNR devices with vacancies in the edge regime turn out to exhibit half-metallic behavior, acting as perfect spin filters for well-defined choices of the strain and the bias [5]. With respect to both the sign and the size, the spin-filtering effect depends sensitively on the device parameters, i.e. the vacancy locations, the bias, and the amount of strain. Similar results are obtained for zGNRs with substitutional transition metal atoms [6]. Further, zGNRs will be discussed in terms of their magnetoresitive properties. Comparison will be made with the respective properties of various types of transition metal dichalcogenides (TMDs), such as MoS_2 and WS_2. On account of their substantial spin-orbit coupling effects, the latter materials are less suitable as spin transport media than graphene, but of major interest as active elements in spintronics networks.

Machine Learning-Based Approach to Predict the Polymorphism of Organic Compounds

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Polymorphism is the capacity of a molecule to be present at the solid state in different conformations and molecular packing.[1] This is a paramount property in the pharmaceutical industry because it determines the stability and the solubility of the drug in the body. In this study, we pursue a novel approach based on machine learning algorithms[2] to predict the likelihood for an organic compound to crystalise in multiple forms. A dataset of molecules was carefully curated from Cambridge Crystallographic Structures Database CCSD and filtered according to the Drug Bank database. A metaclassifier is designed on the obtained dataset to learn the correlation between the compound descriptors and its crystalline form. This study demonstrates that this data mining approach was successful to estimate the number of crystallographic forms on an external validation dataset. These results suggest using this novel methodology to predict the polymorphism of new drugs or not-yet experimentally screened molecules. This promising method can compete with the heavy and slow quantum calculations to predict crystal structures. It is also susceptible to join the experimental high-throughput screening as a guideline to discover new crystallographic forms.

Probing Non-covalent Interactions Driving Molecular Assembly in Organo-electronic Building Blocks

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The present study focuses on if furan and thiophene substituents have an effect on the solid-state properties of and the non-covalent interactions in co-crystals formed between pentafluoro(iodoethynyl)benzene (F_5BAI; XB donor) and a pyridine disubstituted with either a furan or thiophene (PyrFur$_2$ or PyrThio$_2$; XB acceptors). Spectroscopic and thermal analyses of 1:1 mixtures provide indirect evidence of halogen bond (XB) formation whereas X-ray crystallography provides direct evidence that XB and π-stacking are the most prevalent contacts in both co-crystals. Density functional theory computations provide insight into the relative energetics of the various contacts observed in the co-crystals [1-3]. The global hybrid M06-2X density functional is employed in conjunction with a triple-ζ correlation consistent basis set augmented with diffuse functions on all atoms and a relativistic pseudopotential on iodine centers (aug-cc-pVTZ-PP) in order to compute the electronic interaction energies (with and without the Boy-Bernardi counterpoise procedure) of all pairwise contacts that have intermolecular separations of ≤ 5 Å. Within both co-crystals approximately twenty unique contacts are identified that satisfy this distance threshold, where XB and π-stacking interactions are significantly stronger (between -12.0 and -6.8 kcal mol^{-1}) than all other attractive interactions (≤ -2.1 kcal mol^{-1}).
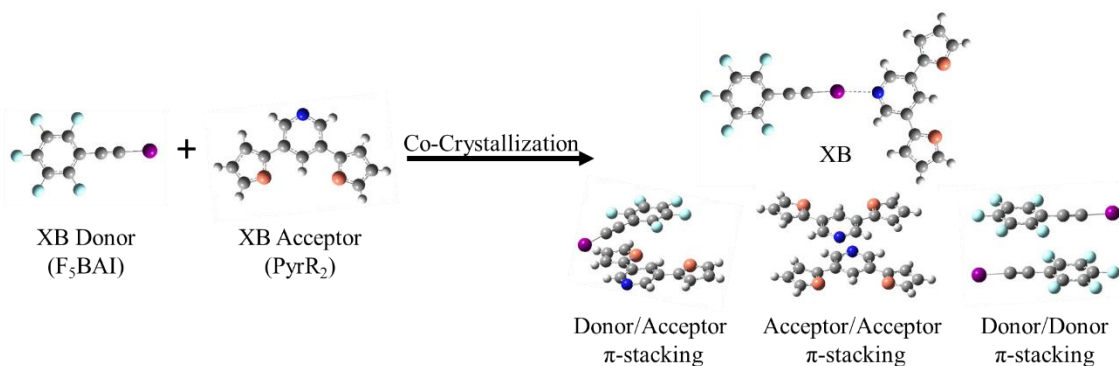
Figure 1: XB Donor (F_5BAI) and the XB Acceptors (PyrFur$_2$ or PyrThio$_2$; where R = Furan or Thiophene) as well as the dominant interactions present after co-crystallization (XB and various π-stacking).

Investigation of the Electronic Structure of Munition Compounds on Corundum-like Oxides

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Arid environments have long been a testing and training ground for novel munitions. However, these activities leave behind unknown quantities of munition residues with unknown impact on local flora and fauna. In particular, arid soil contains Lewis acidic metal oxides which bind and catalyze the electron rich substituent groups commonly found in munition compounds, although the exact mechanisms are poorly understood. The current study remedies this lack of knowledge by utilizing density functional theory (DFT) to explore various orientations of four important munition compounds on the (0001) surface of the corundum-like oxides α-Fe_2O_3 and α-Al_2O_3. Our findings reveal that while α-Fe_2O_3 binds the munition compounds more strongly than α-Al_2O_3, all four compounds experienced elongation of their nitro ($-NO_2$) groups, indicating their susceptibility towards degradation on these surfaces.

Prediction of Munition Adsorption Isotherms on Arid Soil Components

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Arid soils contain a variety of oxide materials *e.g.* corundum (α-Al_2O_3), hematite (α-Fe_2O_3), calcite (β-CaCO3), quartz (α-SiO_2), and albite ($NaAlSiO_4$). In a recent study (Jenness *et al.* PCCP 20, 18850-18861 (**2018**)), we demonstrated how the electronic structure of a munition compounds changes upon adsorption onto corundum and hematite; however, in that study how the temperature and concentration affects the adsorption process was not considered. In the current work, we fill this knowledge gap by utilizing DFT in the construction of an isotherm model. While standard *ab initio* thermodynamic methods are capable of accounting for the effect of temperature, accounting for concentration is a computationally demanding task. However, we have developed a simple linear correction that accounts for concentration and apply it to the problem of TNT and DNAN adsorbing on a variety of soil oxides.

Computer Simulation Study of Differential Capacitance and Charging Mechanism in Ionic Liquid-Based Graphene Supercapacitors

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Ionic liquid based supercapacitors with graphene electrodes are studied via molecular dynamics simulation. As an electrolyte, we consider different types of room-temperature ionic liquids (RTILs). In the first part, we consider various combinations of the same anion ($BF4^-$) with different cations, 1-C_n(n=2, 4, 6)-3-methylimidazolium[1,2] We investigate how the alkyl chain length of the cation affects their interfacial structure and electrical properties for electric double layer capacitors. We first find that cations and anions make layering structures between two parallel electrodes. Cations in the nearest layer orient predominantly in parallel to the electrode. Imidazolium rings of cations form π-stacking with graphene, then the alkyl chains of cations align parallel to the electrode. Differential capacitances in three RTILs are found to decrease with an increase of the magnitude of electrode potentials. The ion size and orientation affect both structure and capacitance behavior. The parallel orientations of cations become stronger with an increase of the alkyl chain length for the considered RTILs. The differential capacitance tends to decrease with raising the alkyl chain length over a wide range of the electrode potential. This is ascribed to a steric effect caused by larger cation size. It is also found that anodic capacitance is higher than cathodic one due to a higher screening efficiency by small anions, and an asymmetry in the peak of capacitance biased to the cathodic side becomes weaker as the alkyl chain length increases. Comparing electrode charge with ion numbers near the electrodes, with respect to their changes in response to the electrode potential, we find that the interfacial layer of the electrolyte mainly governs capacitive behavior of the systems.

In the second part[3], we consider various of anions in RTILs with the same cation, 1-ethyl-3-methylimidazolium(EMIM). In particular, we consider cyano-containing anions, thiocyanate ($[SCN]^-$), dicyanamide($[N(CN)_2]^-$), tricyanomethanide($[C(CN)_3]^-$), and tetracyanoborate ($[B(CN)_4]^-$), respectively. We investigate how electric double layer structure and electrical properties are affected by the structure of cyano containing anions. Differential capacitances in four ionic liquids are found to have a maximum value at negative potential. The maximum capacitances are comparable to each other, but the corresponding potential shifts to the negative side as more cyano groups are attached to the anion. Starting from the interfacial layer, the effects of the further ionic layers on differential capacitance are systematically investigated. Comparing charges of the electrode and those of ionic layers, we find that differential capacitance behavior mainly stems from the ion exchange between electric double layer and bulk region. The ion exchange behaviors are decomposed into cation and anion contributions. The differential charging mechanisms of the system are strongly dependent on the electric potential. The maximum capacitances are consequence of rapid desorption of respective anions.

Characterization of Boron Doped PAH

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The growing interest in the organic materials used in electronics[1–5] towards their general nonlinear optical and electrooptical properties have been the subject of increased attention in the past decade. The traditional inorganic solid-state materials can be replaced by organic or organo-element materials that are easier and less expensive to manufacture[6–8]. Additionally, those materials are more flexible than normal silicon-based structures this feature increases the range of their possible applications[3,11].We propose the use of the boron doped π-conjugated systems [9,10] as nonlinear optical materials. Our study are focused on the boron dopped anthracene dimers. We evaluate the influence on boron doping on the π–π stacking, electron density, and selected optical properties[12].
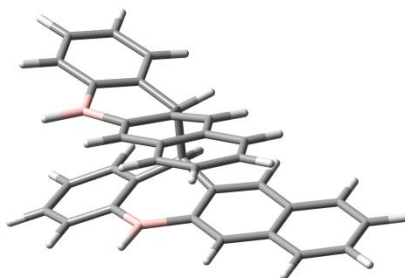
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Exploration of Metal Ion Binding with Homo-dipeptides of Glycine, Alanine and Valine

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Density functional theory (DFT) calculations at the M06-2X/6-311+G(2d,2p) level were performed to understand the binding of homo-dipeptides of three aliphatic amino acids (Ala-Ala, Val-Val, and Gly-Gly) individually with metal ions (Na^+, K^+, Ca^{2+} and Mg^{2+}). Systematic conformational analysis for all three homo-dipeptides were performed initially using MMFF force field implemented in Spartan '16 software package. Geometries of all the conformers for each of the three homo-dipeptides were refined at the HF/3-21G level to find the top three most stable conformers and one least stable conformer. The selected four conformers for Ala-Ala, Val-Val, and Gly-Gly were used to build the complexes with two different types of metal ions: alkali metal cations (Na^+ and K^+) and alkaline earth metal cations (Ca^{2+} and Mg^{2+}). It is known that these metal ions have biological significance. Simple gas phase models give us an idea of the biological functions present [1]. For each of the conformer of Ala-Ala, Val-Val, and Gly-Gly, different possible modes of binding of metal ions were considered in building the complexes. All complexes were fully optimized using M06-2X/6-311+G(2d,2p) level. The data from this computational study provide the knowledge helpful in understanding of metal ion interactions with protein structures. Binding energies with and without basis set superposition error (BSSE) correction were calculated and analyzed. We focused to identify any relationship between the binding energies and structural features of the complexes.

Physics-Based Scale- and Geometry-Consistent Coarse-Grained Potentials

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Modeling biological macromolecules, nanosystems, and interfaces of systems of the two categories requires various levels of detail, from quantum mechanics, through all-atom or atomistic-detailed, coarse-grained approaches, to treatment of a system in terms of classical objects such as springs, geometric shapes or even continuous phases. The consistency between the subsequent levels of reduction of a system representation is essential for successful multiscale modeling, because it is only too easy to ignore the coupling between the parts of a system, which require multibody potentials to be reproduced at lower-resolution level. Recently [1], we developed a general approach to the derivation of effective energy terms in coarse-grained force fields, which is based on the Kubo cluster-cumulant expansion [2] of the potential of mean force of the system under study, where the degrees of freedom omitted in the coarse-grained representation are integrated out [3], and on the Taylor-series expansion of atomic-detailed energy components in the differences of interatomic distances and the distances between the centers of the corresponding coarse-grained sites. The squares of interatomic distances are, in turn, expressed using the trigonometric functions of the angles for the collective rotation of the atoms of the sites about the virtual-bond axes (λ), which are the dominant degrees of freedom to average out. Averaging over the λ angles results in the formulas for the effective energy terms, which are consistent with the Cartesian geometry of a system; in particular, they are gauge-invariant. Moreover, geometrically-consistent functional expressions can be obtained via a simple graphical approach. The method was applied with success to the UNRES model of polypeptide chains [4], improving dramatically its ability to predict protein structures. Moreover, the derived local potentials derived by using this approach from the ab initio energy surfaces resulted in multivariate angle- and dihedral-angle distributions consistent with those extracted from the Protein Data Bank as well as with the details of local geometry of α-helical and β-sheet structures. Local geometrically-consistent potentials were also derived for polysaccharide chains. The proposed approach opens new avenues to systematic derivation of coarse-grained potentials for any systems, with viable extension to treat very low-resolution representation, as far as the continuous phases.

Computational Study of Charge Carrier Mobility in Watson and Crick Deoxyribonucleic Acid (DNA) Bases Pairs for Predictions of Hole Mobility

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Deoxyribonucleic acid (DNA) is the genetic make-up that carries instructions for the development and function of all living organisms. While DNA synthesis have repair mechanisms to correct for mismatch base pairs, however, there are chances in which a genetic mutation can occur. These mutations are the cause of diseases such as, sickle cell disease, Huntington's disease, cancer, and many other diseases in which some of these diseases can be fatal. DNA could possibly be used in high performance devices such as organic field-effect transistors (OFETs), organic light-emitting diodes (OLEDs), and biosensors as the organic semiconductor (OSC) active layer. Using DNA as the OSC layer could have a profound affect in the medical technology field due to allowing early detection for the treatment and prevention of diseases we face in todays' world. In this work, we aim to calculate and increase the charge carrier mobility of these DNA bases.

Molecular Dynamics via Machine Learning: Predicting Energies from Electron Densities

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Density functional theory (DFT) is widely used to calculate the energy of molecular systems and is typically considered to be a computationally affordable electronic structure method. However, using Kohn-Sham DFT in molecular dynamics simulations where the energy must be recalculated at every step is still a costly approach, particularly for periodic materials. Using machine-learned density functionals that map potentials to energies via electron densities allow us to bypass the Kohn-Sham equations in 1D models and in molecular systems. The resulting models enable running molecular dynamics simulations at a significantly reduced computational cost. Examples are presented for isolated molecules, proton transfer reactions, and crystalline solids to illustrate the versatility of this approach.

Study of Thermal Influence on Acetylcholine Ion and DNA Interaction

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The structure of Deoxynucleic acid or DNA is very complex. DNA is a double helix structure that holds the coding for the genetics of all organisms. It is composed of sugar phosphate groups and nitrogenous bases linked together by weak hydrogen bonds. In these nitrogenous bases or base pairs, a purine such as Adenine pairs with a Pyrimidine such as Thymine. The stability of DNA is affected by many factors such as acidity, hydrophobic affects, and temperature. Significant increase in temperature causes the DNA strands to unravel. This process is called denaturation. Also, DNA stability is affected by ions, in the case of this study, Acetyl choline ion. It is understood that the guanine and cytosine bond is stronger than the Adenosine and Thymine bond. However, with the incorporation of the Acetyl choline ion this concept is reversed. This observation was gathered with the experiment at ambient temperature. The goal of this research is to determine whether this same outcome can be seen with temperatures that are higher and lower than that of ambient.

A Combined Computational and Experimental Study on Insensitive Munitions Compounds in Moderately Hard Water

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Alternatives to legacy explosives materials with increased stability against external stimuli are constantly being explored, but environmental interactions and fate of new energetic materials need to be addressed prior to large scale manufacturing. The need for safer munitions materials has led to the development of the class of compounds called insensitive munitions (IMs). We assess the behavior and effects of these compounds in natural water using theoretical and experimental approaches. To investigate the reactivity of IMs, we have undertaken a computational investigation of their interactions in water with environmentally present ions to simulate the reactivity in such environments at the density functional theory level and additionally performed voltammetry experiments for comparison with predicted results.

Red Moon Methodology: A Computational Molecular Technology for Complex Chemical Reaction Systems
- Its Theoretical Treatment and Applications -

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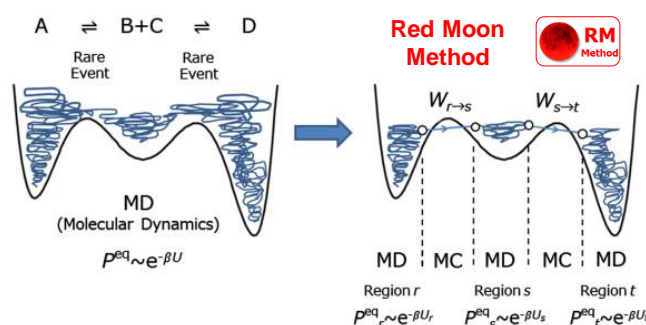*3ESICB, Kyoto University, Kyodai Katsura, Nishikyo-ku, Kyoto 615-8520, Japan*
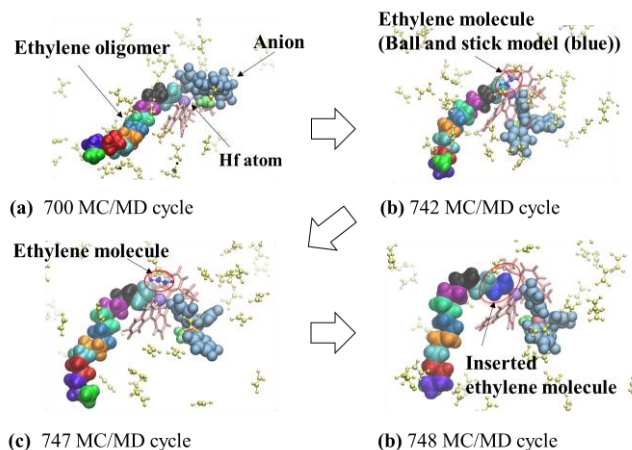**mnagaoka@i.nagoya-u.ac.jp*

Recent development of experimental measurement techniques has made us notice how significant it is to consider chemistry by the number of molecules, not by the amount of substance in mole, leading to the importance of computational chemistry as a molecular science. However, when we try to apply computational chemistry (CC) to diffusion and chemical reactions in "molecular aggregation states" where a large number of atoms and molecules are gathered in condensation, such fact that these phenomena occur only very rarely has made it restrictive or sometime impossible to deal with them by first principles CC methods. Even with traditional classical molecular simulations, it is difficult to determine long-term properties and stereochemical characteristics.

Figure 1. Schematic representation of Red Moon method [1].

Under the circumstances, we have recently developed Red Moon Method (**Figure 1**), a new efficient and practical 'atomistic' simulation method combining Monte Carlo (MC) and molecular dynamics (MD) method with a Rare Event-Driving Mechanism, for large-scale chemical reaction systems [1] and applied successfully to analyze several materials important and valuable in next-generation industrial development [2, 3].

In this talk, several applications of Red Moon Method will be shown from the practical viewpoint of molecular controlling of complex

Figure 2. Polymerization Mechanism by Hf Catalyst

chemical reactions, stereochemistry and aggregate structures [2, 3]. In particular, we would like to take a novel olefin polymerization catalyst (pyridylamido)Hf(IV) complex (**I**), which is activated by a cocatalyst $B(C_6F_5)_3$ to form a cationic active species [4, 5] and explain the role of the counteranion in the reaction mechanism of propylene polymerization [5] (**Figure 2**). Finally, I would like to discuss the microscopic mechanism of chain transfer polymerization of **I** and $ZnEt_2$ in solvent toluene, which is clarified by applying Red Moon simulation to the present system [6].

Conventional Strain Energies of Thiirane, Thietane, Borylthiirane, 2-Borylthietane, and 3-Borylthietane

Summer L. Nash,* Mary Morgan Mohamed,
Shelley A. Smith, and David H. Magers

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A previous study in our group revealed that thiirane (Figure 1) is less strained than cyclopropane and that thietane (Figure 2) is less strained than cyclobutane. A different study of ours revealed that cyclopropylborane is much less strained than cyclopropane. The current study investigates if these effects might be additive. Could a boryl group on thiirane and thietane reduce their strain even more? To answer this question, the conventional strain energies for borylthiirane (Figure 3), 2-borylthietane (Figure 4), and 3-borylthietane (Figure 5) are determined within the isodesmic, homodesmotic, and hyperhomodesmotic models and compared to the conventional strain energies of thiirane and thietane. Optimum equilibrium geometries, harmonic vibrational frequencies, and corresponding electronic energies are computed for all pertinent molecular systems using SCF theory, second-order perturbation theory (MP2), and density functional theory (DFT). The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional and the M06-2X high nonlocality hybrid functional from Thular and Zhao. The basis sets employed are Dunning and coworkers' correlation consistent basis sets: cc-pVDZ, cc-pVTZ, and cc-pVQZ. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Figure 1. Thiirane
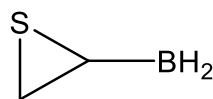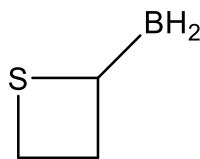

Figure 2. Thietane

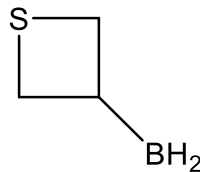Figure 3. Borylthiirane

Figure 4. 2-borylthietane


Figure 5. 3-borylthietane

Prediction of Binding Modes and Affinities of Anti-Tumor Antibiotics with Fullerene as Drug Delivery Vehicle: A DFT Study

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Fullerenes, the third allotrope of carbon after diamond and graphite, have gained paramount research interests in the field of drug delivery applications over the past decade, because of their unique biological activities including toxicity and antioxidant capacity [1-2]. Fullerene-C_{60}, which possesses a unique spherical structure with a strong apolar character, promised to serve as a drug delivery scaffolds through covalent or non-covalent interactions with the bioactive moiety [3-4]. Herein, we have explored the binding characteristics of three anti-tumor antibiotics *viz.* Doxorubicin, Mitomycin and Epirubicin with C_{60} nanocage by performing density functional theory (DFT) based calculations. Stabilities and reactivities of the drug adsorbed fullerene-C_{60} complexes are assessed in both the aqueous and protein core environment. The simulated IR and UV spectra, thermochemical properties, and several chemical reactivity descriptors are analyzed to reveal the nature of the noncovalent interactions between C_{60} and antineoplastic therapeutics.
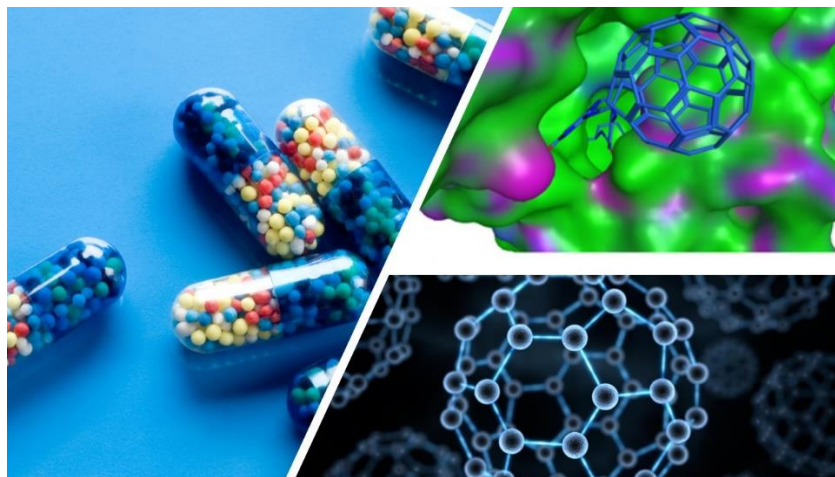
Analysis of the Relative Energies of Isomers of Diphosphetane in Terms of Attractive Versus Repulsive Forces

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Isomers of diphosphetane obviously include 1,2-diphosphetane (Figure 1) and 1,3-diphosphetane (Figure 2). In addition, each of these have *cis* as well as *trans* isomers with respect to the hydrogens bonded to the two phosphorus atoms in each ring. Additional conformations are possible because these hydrogens may be axial or equatorial. Specifically, both axial and equatorial conformations exist for *trans*-1,2-diphosphetane and for *cis*-1,3-diphosphetane. Only one conformation can exist for *cis*-1,2-diphosphetane and for *trans*-1,3-diphosphetane because in these two systems one of the hydrogens must be axial while the other must be equatorial. Optimum equilibrium geometries, harmonic vibrational frequencies, and corresponding electronic energies are computed for all six systems using self-consistent field (SCF) theory, second-order perturbation theory (MP2), and density functional theory (DFT). The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional and the M06-2X high nonlocality hybrid functional from Thular and Zhao. The basis sets employed are Dunning and coworkers' correlation consistent basis sets: cc-pVDZ, cc-pVTZ, and cc-pVQZ. In addition to simply comparing the relative energies, the electronic energies are broken down into the nuclear-electron attraction part and the two repulsive components, the nuclear-nuclear repulsion and the electron-electron repulsion, to gain additional insight into why one conformation is more stable than another. Finally, the individual components of the electronic energy are correlated with average bond distances in these systems. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.
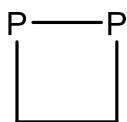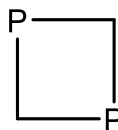

Figure 1. 1,2-Diphosphetane   Figure 2. 1,3-Diphosphetane

Conformational Analysis of Novel Anti-microbial Alkaloid, Solenopsin

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Solenopsin is anti-microbial and anti-inflammatory alkaloid collected from Solenopsin invicta, commonly known as fire ants. The venom can provide defence against microbial pathogens and communication and serve as a novel source of bio-insecticide. In this study, The structure of the Solenopsin compound is being studied via m062x method and 6-31+g(d,p) basis set to find the lowest energy conformations, as they are considered more accurate methods for conformational analysis. The mechanism of bacterial membrane perturbation is studied using these lower energy conformations.

Identification of the stereoisomers of diethyldicyclopentadiene by the ^{1}H and ^{13}C NMR spectra

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The determination of the structure of compounds is one of the most important tasks of organic chemistry. The methods of quantum chemistry are very effective for such purposes. The theoretical study of the NMR spectra has proven to be one of the most commanding methods in structural chemistry and is an exceptional tool for investigations of the structure and conformational properties of the organic molecules.

The following tasks have been accomplished: the experimental investigation of the ^{1}H and ^{13}C NMR spectra of diethyldicyclopentadienes; the theoretical investigation of energetic properties of isomers and the ^{1}H and ^{13}C NMR spectra of diethyldicyclopentadienes; a comparison of the experimental and theoretical results and the identification of regioisomeric diethyldicyclopentadienes.

Calculation of the NMR spectra has been done applying the 6-31G$^{\#\#}$ basis set [1]. Calclations have been performed by the Gaussian 09 program.

During the investigation of the structure of diethyldicyclopentadiene it has been established that each monomer of the molecule exists in one of the three possible isomeric states. As diethyldicyclopentadiene is a dimer, there is a series of twenty-four potential structures. We constructed the set of all possible isomers.
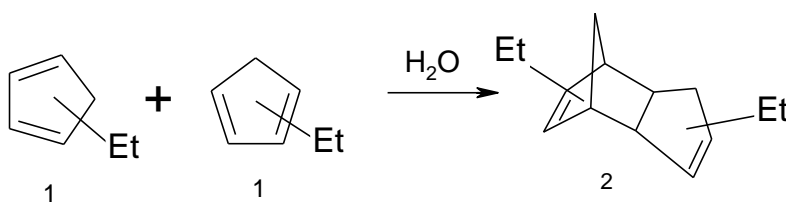
Fig.1. The Diels-Alder dimerization of ethylcyclopentadiene (1)
to diethylcyclopentadiene (2) in aqueous medium

Comparison of the calculated spectra with the experimental data allowed to figure out the structure of the major product and to perform assignment signals of ^{1}H and ^{13}C nuclei.

Binding Energy of Protein Kinase CK2 Complexes with 4'-Carboxyflavonole Derivates. Semiempirical Quantum Mechanical Study

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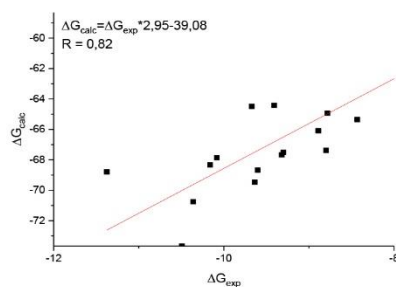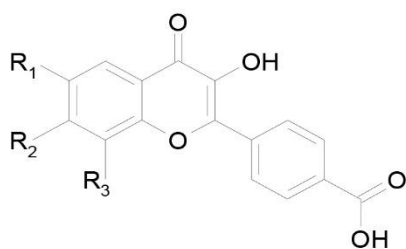[1]Oles Honchar Dnipro National University, Dnipro, 49010, Ukraine
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Presently *in silico* drug design is the promising methodology for the rational construction of new remedies. Number of computational methodologies are used to this aim. The molecular docking and hybrid QM/MM method are the basic approaches for calculation of the protein-ligand (PL) binding free energy. However, these methods are not accurate enough for description of some PL interaction modes. The alternative approach with description of the whole system at quantum chemical level is the semiempirical quantum mechanical (SQM) method.

Here we present the results of the calculations of the binding free energy of seventeen 4'-carboxyflavonole derivates to protein kinase CK2. We have applied the program MOPAC with using of the linear scaling algorithm MOZYME and PM7 method, which among semiempirical approaches, gives the most accurate results for the various types of noncovalent complexes. The influence of solvent (water) has been taken into account by COSMO implicit solvation model.

The crystal structure "CK2α – 6,8-dichloro-4'-carboxyflavonole" (PDB code: 5m4f) has been taken as starting geometry for the construction of the initial complex by the addition of hydrogen atoms and removing of crystal waters except one inner molecule, which forms the hydrogen bonds with inhibitor and Glu 81 in the active site of the protein. The resulting structure has been used as starting point for the modeling of the protein-ligand complexes with the rest of 4'-carboxyflavonole derivatives.

$\Delta G_{calc} = \Delta G_{exp} * 2,95 - 39,08$
$R = 0,82$

Calculated ΔG plotted vs. experimental ΔG
(all in kcal/mol)

Comparison of calculated and experimental ΔG values shows high performance of proposed computational methodology.

Self-Organizing Structures of Interacting Proteins (Cora) By a Coarse-Grained Monte Carlo Simulation

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A transmembrane protein such as CorA for the magnesium channel spans across the membrane with well-defined functions of its inner (iCorA) and outer (oCorA) membrane segments and known to exist as a homo-pentamer. Very recently, we find [1] that the thermal response of icorA differs considerably from that of the outer component ocorA. We further observe [2] that the conformation of iCorA contracts on raising the temperature in native phase, in contrast to its thermal response in denatured phase. The conformational response of the oCorA in its native phase appears to be less organized but differs considerably from that in its denatured phase. A cooperative morphology emerging from interacting proteins is, however, critical in understanding the formation of the ion-channel pathways. Therefore we examine the self-organized structures of proteins (CorA and iCorA) by a coarse-grained model as a function of protein concentration at a range of low (native phase) to high (denature phase) temperatures.

The self-organizing structures show clear distinctions in morphology visually in its dilute concentration from that in the crowded (dense) protein matrix both at low and high temperatures. The morphology is quantified by estimating the effective dimension D of the emerging structures. The effective dimension D of CorA assembly is found to be much lower than that of iCorA segments which remain globular ($D \sim 3$) at almost all length scales in its native phase. CorA proteins remain sparsely extended in random configurations with $D \leq 2$ at almost entire temperature and protein concentrations except at the highest protein concentration considered at low temperature where the most compact morphology is found with $D \sim 2.6$. The radius of gyration of the protein CorA does not show much variation with the protein concentration at low temperatures while that of iCorA increases with the protein concentration systematically in its native phase. Higher structural response of the inner-segments in its native phase may be more conducive to self-organizing pathways due to protein-protein interactions.

A Comparison of Electronic Properties of Conformers of Insensitive Munition 4,6-bis(nitroimino)-1,3,5-triazinan-2-one (DNAM) – A Computational Study

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In order to minimize unintentional detonation, current munitions research has focused on the development of chemical compounds that are insensitive to external stimuli whilst maintaining their effectiveness. The compound 4,6-bis(nitroimino)-1,3,5- triazinan-2-one (DNAM) has recently garnered attention as a potential candidate for such insensitive munitions (IMs). DNAM exists in several tautomeric forms, and we have focused on the nitroimino-keto (NIC) form which has been identified as the most stable tautomer. Furthermore, we explore three different conformers of the NIC form in both the gas phase and bulk water solution via implicit solvation using the conductor-like polarizable continuum model (CPCM) and density-based solvent model (SMD). We employed both density function theory and MP2 theory methods; the relative energies, ionization potentials, electron affinities, redox potentials and pK_a values will be discussed.

Towards computational risk assessment of ionic liquids

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and T. Puzyn*

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The number of research papers discussing unique properties and novel applications of ionic liquids (ILs) systematically increases. ILs are considered as efficient solvents for many chemical processes due to their low vapor pressure, high ionic conductivity, low flammability, ability of dissolving a wide range of compounds, high thermal stability and tailored polarity (hydrophobicity). Chemically, an ionic liquid is a combination of a usually large cation and a smaller anion (Fig.1.). The properties of ILs can be precisely designed by appropriate modifications of the cation's and/or anion's structure [1].
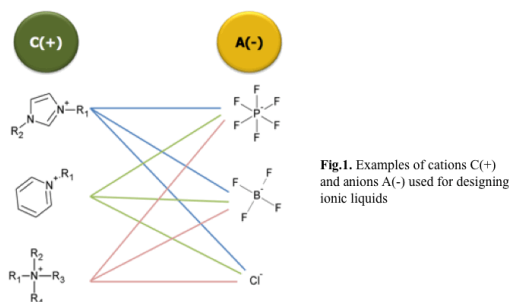
Fig.1. Examples of cations C(+) and anions A(-) used for designing ionic liquids

However, there is a serious concern on safety of newly designed ILs to human health to the environmental organisms. The procedures of risk assessment should include both evaluation of the hazard and the exposure.

Nowadays, computational methods are widely used for supporting the risk assessment of new chemicals. The array of available methods includes Quantitative Structure-Activity / Structure-Property Relationships (QSAR/QSPR) modeling and Multimedia Mass-balance (MM) modeling [1, 2]. Unfortunately, such methods have been unavailable so far for ILs because of many methodological and technical problems.

In this presentation, the current achievements and further challenges for QSAR/QSPR and MM for ionic liquids will be discussed. A special focus will be put on recently developed ILsTOX database containing the experimentally obtained and predicted data for risk assessment of ILs [3]; the contributions related to the appropriate way of calculating molecular descriptors for ionic liquids [4-6]; new tools for exposure assessment of ILs including ILPC screening tool [7] and AquaBoxIL toolbox for MATLAB [8, 9]; QSAR models developed for predicting ILs toxicity [10] and TRIC index for toxicity prioritization of cations [1] and, finally, RExIL software tool – Risk Explorer for Ionic Liquids [11].

PAHs (Polycyclic Aromatic Hydrocarbons)

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Polycyclic Aromatic Hydrocarbons (PAHs) simply put are a group of different chemicals released as the result of the incomplete combustion of organic materials. Their production can be stemmed from the process of burning: coal, gasoline, trash, tobacco, or wood. The purpose of this research is to assist with the determination of the reaction pathway of 3-Nitrofluoranthene into a carboxylic acid derivative through UV/Vis excitation. These compounds depending on its orientation can be either beneficial or harmful to living organisms. PAH's can be found in medicines along with being components of dyes, plastics, and pesticides. The danger found with compounds comes from their reactive metabolites (electrophilic species) can bind to molecules like DNA which can lead to cancer. The development of cancer is the result of extended exposure to PAHs in which the DNA covalently binds to a toxigenic PAH. Contact with these molecules are numerous but the most common including ingestion, inhalation, or dermal contact. After chronic exposure various bodily systems will begin to be affected; systems such as pulmonary, gastrointestinal, renal, and dermal. However, the positive aspects of PAH's are that they are used in medicines for skin diseases like psoriasis. Computational methods will be implemented in the analysis of the hypothesized degradation pathway. Density Functional Theory (DFT) calculations were executed to observe and collect UV spectra and excitation energies.

Solvation of Isoelectronic Halide and Alkali Metal Ions by Noble Gas Atoms

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Alkali metal cations (M^+ = Li^+, Na^+, K^+, and Rb^+), as well as their corresponding isoelectronic atomic anions (X^- = H^-, F^-, Cl^-, and Br^-) were solvated with 1 - 6 argon atoms (i.e., M^+Ar_n and X^-Ar_n where n = 1 - 6). Full geometry optimizations were performed using the MP2 electronic structure method with a series of correlation consistent basis sets augmented with diffuse functions on argon and the anions (aug-cc-pVXZ), whereas weighted core valence basis sets were used for the cations (cc-pwCVXZ). The basis sets for a particular cluster are, hereafter, simply denoted as XZ where X = T and Q. Harmonic vibrational frequency computations were performed to characterize the nature of each stationary point on the MP2/TZ potential energy surface. A series of single point energies and scans were also performed using MP2, CCSD, and CCSD(T) methods with basis sets as large as 5Z for the smaller clusters to gauge basis set and electron correlation effects. Previous work on the cation clusters [1,2] helped guide our efforts to also determine the lowest energy structures for the anion systems and additional cation systems. These computations were performed to explore similarities and differences between the isoelectronic cation and anion pairs (Li^+ vs. H^-, Na^+ vs. F^-, K^+ vs. Cl^-, and Rb^+ vs. Br^-).

Indoline Based Photo Efficient Dye-sensitizers with D-A-π-A Framework: A Computational Approach

Juganta K. Roy, Supratik Kar, Jerzy Leszczynski

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A good number of research efforts has garnered on the advancement and understanding processes of converting and storing solar energy in a specific molecular system. Seven D-A-π-A based Indoline (IND) dyes designed via Quantitative-Structure Property Relationship (QSPR) modeling and have been investigated theoretically in depth to evaluate their prospect of application in future dye-sensitized solar cells (DSSCs). Our proposed seven lead dyes have D-A-π-A framework and are characterized by the encouraging PCE values. Optoelectronic properties of the isolated dye and dyes adsorbed on a TiO_2 cluster that simulates the semiconductor explored with the implication of DFT and TDDFT methods. Considering the balance between the V_{OC} and J_{SC} along with the all calculated characteristics, the IND3, IND5, and IND10 are the most suited among the designed dyes to be used as potential candidates for the photo efficient DSSCs. The present study provides rational molecular design followed by the exploration of photophysical properties to be used as a valuable reference for the synthesis of phot-efficient dyes for DSSCs.

How Do Amine Bridges Affect
Conjugation in Monomacrocyclic Dendrimer Precursors?

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Due to previous work conducted by the Mississippi College Computational Chemistry Group, it was determined that when forming monomacrocyclic dendrimer precursors, flat, two-dimensional systems seem to occur more often when 2-pyridinyl groups are utilized. This project originated when the Mississippi College Organic Research Group (MC-ORG) synthesized dendrimer precursors that were not as flat as desired. Dendrimers need this "flat" orientation in order to retain their conjugation, and therefore, their light harvesting properties. The MC-ORG dendrimers being synthesized contain ethynyl units that are theoretically being locked in place by ether connections. The goal of this research is to determine whether reducing the hydrogen interactions in the bridge between the 2-pyridinyl rings would further assist in forming flat dendrimers and retaining conjugation. To do this, amine bridges are placed between the 2-pyridinyl groups that will theoretically lock the ethynyl bridges in place and form flat dendrimers (Figure 1). This amine connection is studied with different carbon lengths in the bridge and in the positions both *ortho* and *meta* to the ethynyl groups. To investigate these questions, optimum structures are computed at the SCF and DFT levels of theory. The functionals employed are B3LYP, M06-2X, and ωB97XD. The basis sets employed are Dunning and coworkers' correlation consistent basis sets, cc-pVDZ and cc-pVTZ. All calculations use correlation consistent basis sets. Finally, time-dependent DFT calculations are used to investigate the UV-Vis spectra to determine if these various amine connections will improve conjugation within the structure. In the future, NICS calculations will be conducted to determine the aromaticity, and therefore further prove if conjugation is retained.
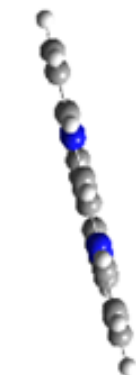

Figure 1: Pyridines with Meta Alkenyl Diamino Bridge

First-principles calculations of the electronic structure and optical properties of α-Al$_2$O$_3$ thin film under uniaxial strain

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Aluminum oxide exhibits several crystallographic polymorphs; and its thin and thick films show promising technological applications range from optoelectronic devices to catalysis, thermal barrier, and wear resistant; because of their excellent properties such as high mechanical strength, high electrical resistance, and high dielectric constant [1]. Also, under high pressure conditions there are several potential technological applications for aluminum oxide [2]. As a typical ceramic material, sapphire (α-Al$_2$O$_3$) holds a combination of interesting properties including hardness, high wear resistance, chemical inertness, as well as optical transparency from the near infrared through the visible region into the ultraviolet. Due to its importance for optoelectronics, several investigations have been devoted to developing a fabrication procedure for aluminum oxide thin films with enhanced mechanical and optical properties. It has been shown that aluminum oxide thin films prepared under optimized conditions of oxygen partial pressure exhibit good optical properties. Despite the technological importance, there is no more comprehensive experimental or theoretical study that provides clear explanation behind the reduction of energy band gap value obtained for thin film alumina. These observations motivate us to investigate the mis-match strain effect on the electronic structure and band gap of Al$_2$O$_3$ thin film.

In this context, we have explored the structural, electronic, and optical properties of Al$_2$O$_3$ thin film under uniaxial strain by conducting density functional theory (DFT) based computations. The key goal is to provide fundamental insights that connect the electronic structure and optical properties of the multilayered system with its mechanical properties. The optical properties including dielectric function, refractive index, extinction coefficient, and reflectivity have been estimated under uniaxial strain ranging from 0-18%, and the impact of uniaxial strain on the band offset is also examined. The dynamic stability of the Al$_2$O$_3$ thin film has been verified by calculating phonon band dispersions and density of states under different strain rates.
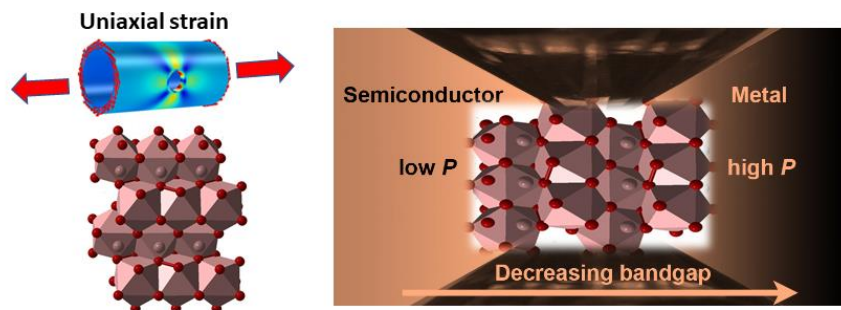
Computational Development of an Organic Sensor and Sensor Characteristics

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Water quality is important for sustaining life and for proper functioning of the ecosystem. Our ecosystems yield food and economic development for many along the Southern Coastal area. It is critical to detect and remove pollution before our ecosystems are destroyed. However, there remains very few options to detect these changes within the water system. One such change that would be important to detect are the rising carbon dioxide levels in water. When the oceans absorb CO_2, the chemical reaction that takes place produces carbonic acid (H_2CO_3), which increases the acidity (lowers the pH) of seawater. Many scientists believe that the decreasing pH in the oceans interfere with the ability of certain marine animals, such as corals and other calcifying marine organisms, to make their skeletons and shells from calcium carbonate minerals. There are several potential compounds that can be used to detect CO_2 due to the binding properties of the molecule. In this work, we will explore the absorption of carbon dioxide in water with a well-known CO_2 binding compound known as Triazabicyclodecene (TBD). TBD has been chosen to promote the insertion of CO2 because it has been proven to strongly bind CO2. Upon learning this, several experimental nitrogen base compounds were created and their pk values were calculated and compared to that of TBD.

Ab Initio Calculations with Chemical Accuracy
for Molecule - Surface Interactions and the Performance of DFT+Dispersion

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The *ab initio* prediction of molecule-surface interaction energies with hundreds of atoms with an accuracy that is comparable to experiment is a challenging problem of computational quantum chemistry. We apply a hybrid method [1] that uses MP2 at the reaction site and DFT-dispersion for the full periodic structures. We perform structure optimization at this level, and – as single point calculation – perform CCSD(T) calculations for smaller cluster models.

With this *hybrid MP2:DFT-D + □CC* approach we calculate adsorption energies for ten systems for which reliable experimental data were available:
(i) adsorption of CO,[2] as well as CH_4 and C_2H_6[3] on the MgO(001) surface,
(ii) adsorption of H_2,[4] CO,[5] CO_2[6] and CH_4[7] in metal-organic frameworks (MOF),
(iii) adsorption of small alkanes in zeolite H-Chabazite[8]

We show that the results agree within chemical accuracy limits with "experimental" reference energies. The latter are derived from measured enthalpies using zero-point vibrational energies and thermal energies obtained with PBE+D.

$$\Delta E\,(Ref)\ = \Delta H_T\,(Exp) + RT\ - \Delta E_{therm}\,(DFT\text{-}D) - \Delta E_{ZPV}(DFT\text{-}D),$$

We use these "experimental" reference energies to test different ways of taking within DFT dispersion into account as implemented in the VASP code:
(i) Parametrized $1/r^6$ terms "D2" and "D3" after Grimme, and after Tkatchenko/ Scheffler "TS"
(ii) Many body approach of Tkatchenko, including "HI" and "FI" variants
(iii) van der Waals functionals, vdW-revPBE and vdWoptB86b

The best performing ones were PBE+D2, PBE+MBD/HI and PBE+MBD/FI with mean unsigned errors of 6.5, 6.0 and 5.7 kJ/mol, respectively.

Dynamic Phase Partitioning During Ester Nitration in a Tertiary Solvent

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Phase dynamics are an important part of chemical synthesis pathways for many nitrate ester compounds. In this study, the interactions of glycerin compounds at different levels of nitration in dichloromethane, glycerol, and nitric acid solvents were characterized to predict trends and elucidate ways to improve control of the reaction. Molecular dynamics simulations provided atomistic detail of the biphasic separation, phase partitioning of solutes, transport, and solute-solvent interactions. The data is enumerated and discussed in terms of how processing conditions would be expected to impact the overall reaction dynamics.

The Effects of Ions and Humic Acid on Munition Compounds in Natural Waters

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In natural waters, there are many factors such as surfaces and solvated ions that contribute to the degradation and behavior of munition compounds in the environment. In the aqueous phase these effects were characterized for 8 common ions using MD and QM/MM approaches. For the adsorbed phase, humic acid (HA) substances comprise the majority of organic carbon content in natural soil environments and play significant roles in the retention and degradation of munition compounds used at testing and training ranges, manufacturing sites, and storage facilities. HA model has been used with molecular dynamics - thermodynamic integration (MD-TI) and density functional theory (DFT) methods to characterize the changes in munition binding energy, ionization potential, and electron affinity observed when munition compounds are bound with HA compared to when in water. Several munition compounds (MC's) were studied including insensitive munitions and legacy high explosives: DNAN, $[DNi]^-[NH4]^+$, nMNA, NQ, NTO (neutral and anionic forms), TNT, and RDX. The results show that HA readily binds most MC's and can act as both a sink and source for electron density thus buffering MC's against both oxidative and reductive attack. Data shows how HA would have an impact on fate and transport of MC's in the environment.

Electronic Structure and Chemical Properties of Long-Bonded Isonitrosyl Compounds

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Volatile organic compounds (VOCs) are the critical ingredients of atmospheric pollution. VOCs enhance the ozone formation in the global troposphere, stratospheric ozone depletion, long range transport of chemicals in atmosphere, acid deposition and, ultimately, contribute to the global climate change.[1] The VOCs enter the atmosphere from anthropogenic and biogenic sources, and trace amount of VOCs can be formed as products of the atmospheric transformations of other VOCs. The major classes of anthropogenic sources are alkanes, alkenes, aromatic hydrocarbons, and oxygenated compounds.[2] Interestingly, photodissociation or thermal dissociation of VOCs produce highly reactive and unstable species. For example, a recent study showed that photo dissociation of HONO might lead to formation of unusual iso-coordinated recombination product of HO• and NO•.[3,4] The high-level ab initio electronic structure calculations of HO—ON showed that it could exist as a relatively stable molecule (the O—O bond dissociation energy is 8 kcal/mol)[3] despite its remarkably long (1.9 Å) central O–O bond which may lead to an unusual behavior of HO—ON.[4] Similarly, such long-bonding can be seen in methoxy iso-nitrosyl (CH_3O—ON) which was predicted to be an intermediate of important atmospheric reaction of photodissociation of alkyl nitrites.[5]

Even though many studies are performed to rationalize the formation of CH_3O• + NO• and CH_3• + NO_2•,[5-7] the dynamics of long-bonding phenomena in CH_3O—ON is yet untouched. Our study was conducted to investigate this iso-coordination long-bonding property in methoxy iso-nitrosyl and address the question how long-bonding influences the dynamics of formation of CH_2O+HNO to CH_3O•+ NO•. Specifically, we have computationally analyzed the formation of CH_2O+HNO by two possible path ways as shown in Fig. 1.
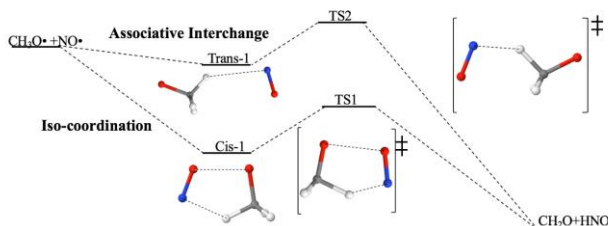

Fig.1. The two possible pathways of H transfer reaction

According to the results that were obtained at the CCSD(T)/aug-cc-pVTZ level theory, iso-coordination pathway is thermodynamically more favorable with respect to the associative interchange pathway by 15.3 kJ/mol which is shown in the top part of Fig.1.

To further examine these results, we proceeded with the Atoms-In-Molecule (AIM) electron density topological studies. By comparing the structural features of reactants, intermediates, and

transition states, we noticed that the peroxide bond in the transition state **TS1** has a polar character. As compared with the isolated methoxy radical, the methoxy moiety in **TS1** gains partially negative charge, which facilitated the formation of pi bonding between C and O atoms in the formaldehyde moiety. [8] This extra negative charge gained by methoxy O atom reduces the activation barrier between **cis-1** and **TS1** (Fig.1), which leads to a kinetically favorable pathway. According to the AIM topological analysis, there is a critical point located between the two O atoms in **TS1** indicative of the presence of iso-coordinated long-bonding between the two O atoms, similar to that in the HO—ON system. Furthermore, the critical point is located closer to the O atom in nitrogen oxide than to methoxy O atom, which signifies the polar character of peroxide bond in **TS1** and the catalytic behavior of iso-coordination pathway.

The reaction shown in Fig.1 involves the transfer of H atom, which has relatively low electronegativity. To address the question how a similar reaction proceeds for the case when the transferred atom has high electronegativity, we studied the F atom transfer in the CF_3O—ON system. We use the same methods to evaluate all the reactants, intermediates, transition states, and products as in CH_3O—ON. When comparing the iso-coordination pathway between CF_3O—ON and CH_3O—ON, we observed the increase in activation barrier for the CF_3O—ON system. Surprisingly, the barrier was increased despite that the bond polarity was even more pronounced in CF_3O—ON. Hence, AIM calculations and electron density topological study analysis will be conducted to describe this phenomena.

Our results agree well with the computational study that was conducted by Bofill, Anglada et al in 1999, [8] in which they studied the interaction between methoxy radical and O_2 molecule. They also observed that iso-coordination between the oxygen atoms assisted the H atom transfer between C and O atoms were greatly assisted.

In conclusion, our study demonstrates that the long-bonded iso-coordination between a molecule and a radical is not an uncommon chemical bonding motive. Furthermore, such long-bonding iso-coordination can significantly affect the mechanisms by lowering the activation barrier of rate limiting steps.

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Evaluating Photocatalytic Active Sites as Function of Polarization, Level Alignment and Spontaneous Dissociation of Hydroxyl Groups at Perovskite Oxide Surfaces

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SrTiO3 is a high efficient photocatalyst under UV irradiation. It is also a perovskite oxide, which allows it to be epitaxially grown with well-defined surfaces. This control makes of SrTiO3 and other perovskite oxides ideal platforms to study the atomistic mechanisms of photocatalytic water oxidation. PbTiO3 is a ferroelectric perovskite oxide that also absorbs in the UV range. In addition to controlled epitaxial growth, it is possible to control its ferroelectric polarization at the nanoscale. We apply this control to investigate the interplay between polarization and surface termination on the photocatalytic activity of these two materials using the photocatalyzed reduction of silver-nitrate solution to silver as a proxy reaction for evaluating water oxidation. We also perform ab initio molecular dynamics simulations of liquid water on all the experimentally grown perovskite oxide surfaces. Our results clearly evidence the critical role played by surface termination and polarity on water dissociation into proton and hydroxyl ions at the surfaces. These surface hydroxyl ions are the initial species in the water oxydation cycle. Our results show that in SrTiO3 the oxidation and reduction reactions occur at the boundary between surface termination changes. Water oxydation occurs primarily in SrO terminated surfaces, where the overpotential for the photo-generated holes is larger. The silver reduction occurs at the TiO2 edges.

We hypothesize that these results are consistent with a small spatial extent of the photo generated electron-hole pairs coupled to the localization of the photogenerated hole on the SrO surface. To test this hypothesis, we have theoretically evaluated the dissociation and overpotential properties of a series of alcohols in these surfaces. We also performed the same experimental photocatalytic procedure on aqueous solutions of these alcohols. Our results show indeed that silver is still only deposited in the vicinity of SrO surfaces and even more that there is a direct correlation between the amount of silver deposited and the overpotential of the de-protonated Oxygen bound to the SrO surface. This confirms the essential role played by surface acidity on the photocatalytic process.

Binding energy of protein kinase CK2 complexes with 4'-carboxyflavonole derivates. Semiempirical quantum mechanical study

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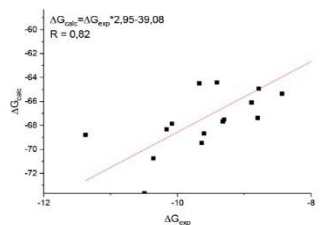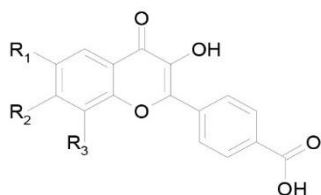1. Oles Honchar Dnipro National University, Dnipro, 49010, Ukraine
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Presently *in silico* drug design is the promising methodology for the rational construction of new remedies. Number of computational methodologies are used to this aim. The molecular docking and hybrid QM/MM method are the basic approaches for calculation of the protein-ligand (PL) binding free energy. However, these methods are not accurate enough for description of some PL interaction modes. The alternative approach with description of the whole system at quantum chemical level is the semiempirical quantum mechanical (SQM) method.

Here we present the results of the calculations of the binding free energy of seventeen 4'-carboxyflavonole derivates to protein kinase CK2. We have applied the program MOPAC with using of the linear scaling algorithm MOZYME and PM7 method, which among semiempirical approaches, gives the most accurate results for the various types of noncovalent complexes. The influence of solvent (water) has been taken into account by COSMO implicit solvation model.

The crystal structure "CK2α – 6,8-dichloro-4'-carboxyflavonole" (PDB code: 5m4f) has been taken as starting geometry for the construction of the initial complex by the addition of hydrogen atoms and removing of crystal waters except one inner molecule, which forms the hydrogen bonds with inhibitor and Glu 81 in the active site of the protein. The resulting structure has been used as starting point for the modeling of the protein-ligand complexes with the rest of 4'-carboxyflavonole derivatives.

Calculated ΔG plotted vs. experimental ΔG
(all in kcal/mol)

Comparison of calculated and experimental ΔG values shows high performance of proposed computational methodology.

Photochemical and Thermochemical Degradation of Nitroguanidine: A Computational Chemistry Investigation

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Development of low vulnerable munitions without compromising their explosive properties has been an important area of research. Nitroguanidine (NQ) is one of the important insensitive munitions compounds currently being used in various insensitive munitions formulations. NQ degrades in the environment, and cyanamide has been suggested to be the end product of NQ degradation. Previous experimental studies of NQ photolysis have shown a number of different products, yet the reports are often in disagreement with regard to kinetics and product distribution. Scission of the N—NO$_2$ bond has been proposed as the primary reaction, and evidence exists showing this to be a homolytic cleavage. We have used Density Functional theory utilizing M06-2X functional and 6-311G(d,p) basis set to investigate detailed mechanisms of degradation of these compounds in the water solution. Higher level of augmented quadruple Dunning's correlation consistent basis sets aug-cc-pVQZ were also used in some cases for comparison with results obtained at the 6-311G(d,p) basis set. The force constants were determined analytically in the analysis of harmonic vibrational frequencies for all of the complexes. An intrinsic reaction coordinate (IRC) analysis was carried out to ensure that each transition state links to the corresponding reactants and products (both as local minima on the potential energy surface). The conductor-like polarizable continuum model (CPCM) was employed to simulate the entire reaction in water solution. The Gaussian-09 package of programs was used for all computations. Our theoretical calculation revealed that degradation pathway has a mixed mechanism including both photolysis and chemical hydrolysis processes.
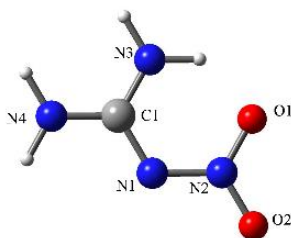
Structure of NQ

Enthalpies of Formation of Methyl Derivatives of Furan, Pyrrole, Oxazole, Isoxazole, and Imidazole by Homodesmotic Reactions

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Furan, pyrrole, oxazole, isoxazole, and imidazole are all examples of heterocyclic aromatic compounds (Figure 1). They and their derivatives have a variety of uses. 2,5-dimethyl-furan has been proposed as a possible biofuel; pyrrole is a component of both heme and chlorophyll; ibotenic acid, a derivative of isoxazole, is a powerful neurotoxin; and histidine is a derivative of imidazole. In the current study, we focus on the computation of the standard enthalpy of formation of methyl derivatives of these aromatic heterocycles by homodesmotic reactions. In homodesmotic reactions the number and types of bonds and the bonding environment of each atom are conserved. The enthalpy of all the reactants and products in each homodesmotic equation is computed using SCF theory, second-order perturbation theory (MP2), and density functional theory. The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ωB97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets, cc-pVDZ, cc-pVTZ, and cc-pVQZ. From the resulting enthalpy of reaction, the desired enthalpy of formation is determined by use of reference values for all other systems in the reaction. Thus, the calculation of atomization energies is avoided. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.
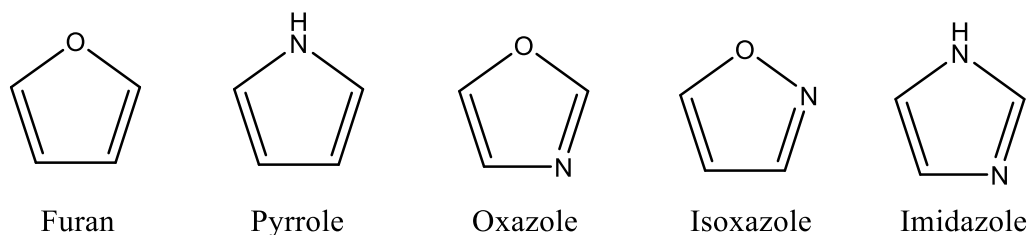

Figure 1. Parent heterocyclic aromatic compounds

A Computational Study of Ionized Water Clusters (H$_2$O)$_n$, n=1-15

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Long-term duration space travel poses a great threat to the health of astronauts. Scientists have proven that radiation is harmful to the body and briefly studied the biological damage that can occur. Consequently, biological countermeasures and shielding methods are being developed. However, to gain insight on specific criteria for radiation shielding and biological protection, one must first analyze the effects of radiation on the body. Because the cell is mainly composed of water, the probability that radiation will interact with water is high. Therefore, an analysis of water's response to radiation at a molecular level is required. Calculations have been performed using the 6-31 +g(d,p) basis set and the density functional, M06-2X, to optimize the most stable geometries of water clusters (H$_2$O)$_n$, n=1-15.

Investigating the Retention of Conjugation in Monomacrocyclic Dendrimer Precursors Using Phenyl and 2-Pyridinyl Groups

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Conjugated dendrimers have been studied for their use in preparing photoreactive materials and for their light harvesting properties. The Mississippi College Organic Research Group (MC-ORG) has been attempting to design and prepare flat, two-dimensional dendrimers. It has been found that when twisting occurs about the single bonds of the dendrons, there is a decrease in energy transfer which results in a loss of conjugation. This loss of conjugation is undesirable since conjugated dendrimers are of interest due to their use in preparing photoreactive materials and for their light harvesting properties. These "flat" dendrimers should retain their conjugation due to the ethynyl units theoretically being locked in place by ether connections. These ether connections are created during an intermediate step when a monomacrocyclic dendrimer is formed. The goal of this research is to assist MC-ORG in project development by determining whether a one, two, three, or four carbon connection would form an ether bridge in positions both *ortho* and *meta* to the ethynyl groups without twisting of the ethynyl units. It will also be determined if replacing the phenyl groups (Figure 1) with 2-pyridinyl groups (Figure 2) will reduce the amount of twisting due to hydrogen interaction on the interior of the dendrimer precursor. The functionals employed are B3LYP, M06-2X, and ωB97XD. The basis sets employed are Dunning and coworkers' correlation consistent basis sets, cc-pVDZ and cc-pVTZ. All calculations use correlation consistent basis sets. Finally, time-dependent DFT calculations are used to investigate the UV-Vis spectra to determine if these various ether connections will improve conjugation within the structure. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.
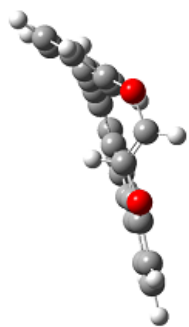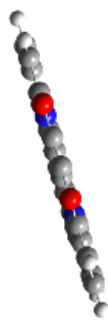
Figure 1: Benzenes with Meta Diethenyl Bridge

Figure 2: Pyridines with Meta Diethynyl Bridge

In silico photolysis and Fenton oxidation of NTO (3-nitro-1,2,4-triazol-5-one)

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NTO (3-nitro-1,2,4-triazol-5-one) is an important energetic material for military applications. It may find its way to the environment during manufacturing, transportation, storage, training, and disposal. Concentration of NTO may be significant in water due to its high solubility (16.642 mg L^{-1}). Photolysis is one of the major abiotic processes affecting the transformation of energetic compounds in the surface water. Experimental data showed that TiO_2-catalyzed photo-degradation leads to the complete mineralization of NTO. Fenton oxidation offers an efficient cost-effective method for NTO remediation. It was suggested that these remediation methods based on interaction of NTO with hydroxide radical, formed from water or hydrogen peroxide under metallic catalyst action. The main observed products were nitrite, nitrate, carbon dioxide. To shed light on reaction pathways for NTO decomposition we performed a detailed computational study of possible mechanisms for interaction of NTO with hydroxide radical using the PCM(Pauling)/M06-2X/6-311++G(d,p) approach. Predicted products are in good agreement with experimental data.
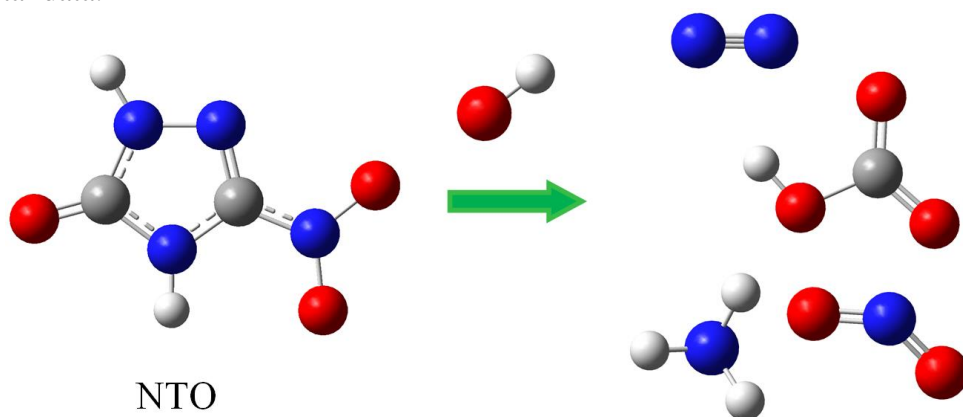
NTO

# Computational Study on Molecular Imprinting of S-Propranolol Towards Designing Transdermal Delivery System

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S-propranolol is a medication that is used to treat high blood pressure, performance anxiety, and also to prevent migraine headache. Currently its main delivery route to the patient's body is oral or intravenous. However, because of existing side effects (nausea, abdominal pain, and constipation) we propose an alternative way for administration of s-propranolol in a form of the transdermal patch. In addition to minimizing side effects, the patch can be administered to unconscious patients or used in the situations where performing injection is not possible. Transdermal patch can be easily stored, transported, and administered to the patients.

Molecular imprinting is the technique that allows encapsulation of the molecule of interest, a template, into the polymer matrix. Due to the type of interactions between MIP and template, the former can easily be removed from the polymer cavity and then rebinded. MIPs are widely used for detection, selectivity, separation of racemic mixtures, and recently for a drug delivery purposes.

Our project focuses on the designing a molecularly imprinted polymer that acts as carrier for the slow release of the s-propranolol. Our goal is to understand the binding process between S-propranolol and methacrylic acid, MAA, based MIP towards its application as a transdermal patch. We apply *ab initio* methods to evaluate the template binding/release dependence on the solvent, temperature and pH fluctuations. Our results provide molecular level of understanding of the s-propranolol release process from MIP cavities.
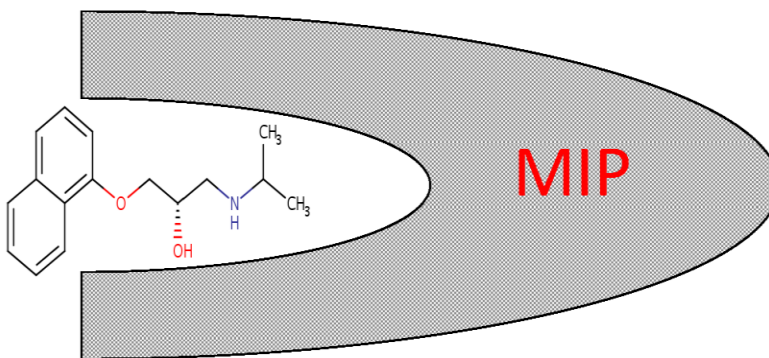
Fig. 1. Schematic representation of **S**-Propranolol encapsulated in MIP

A Tale of Water and Halogens and the Toolbox Needed to Unveil their Narrative

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The coming of age of computational chemistry craftsmanship is quite evident: the number of macroscopic phenomena we understand from their molecular interactions increases continuously. Some of these endeavors have provided sound explanations of complex biological mechanisms, properties of man-made materials and, more recently, spectroscopic properties of condensed phases.

We have combined approximate methods and refined *ab initio* methodologies to follow the interaction between water and halogens, chlorine and bromine specifically, from gas-phase clusters[1] to the halogen hydrates[2]. We were able to identify the physical ingredients of the spectroscopic signature of halogens in different aqueous media. The accurate experimental measurements of the absorption spectra of chlorine and bromine clathrate made by the groups of Janda and Aapkarian[3] were tests of the suitability of each of the theories and methods used for the theoretical description of these systems thus, enabling the continuous refinement of the semi-empirical models employed and the choice of levels of theory needed for their study. In this talk I'll present the patchwork created with different tools where the nature of the halogen – water interaction is changing and at the same time, modulates the spectroscopic response from phase to phase.

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General-Order Spin-Free Coupled-Cluster methods

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A general-order coupled-cluster method is formulated using spatial orbitals, for both closed- and open-shell states. For open-shell states, we extended the partial-spin adaption scheme [1,2] to the full configuration-interaction limit by systematically improving the spin adaption. Double-coset techniques was used to simplify the canonicalization procedure [3,4]. Additionally, the relation between partial spin adaption and genialized normal ordering [5] was discussed.

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Structural and Binding Insights into HIV-1 Protease and P2-Ligand Interactions through Molecular Dynamics Simulations, Binding Free Energy and Principal Component Analysis

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HIV-1 protease (HIV-1 PR) plays an important role in viral replication and maturation, making it one of the most attractive targets for anti-retroviral therapy. It is important to design new effective inhibitors that combat drug resistance in mutant HIV-1 PR variants. In this work, we explored the interactions between two P2-ligands (Darunavir, DRV/TMC114 and amino-bis-tetrahydrofuran derivative, 4UY) with wild type (WT) HIV-1 PR and mutated p20 and p51 variants through molecular dynamics (MD) simulations, binding free energy calculations, and principal component analysis (PCA). DRV or 4UY binds with HIV-1 PR via both hydrogen bond and hydrophobic interactions in the active site, flap and 80s loop region. Importantly, 4UY interaction with Gly48/Gly48′ in the flap region of the HIV-1 PR makes it more stable than the DRV. Calculated Molecular Mechanics/Poisson-Boltzmann Surface Area (MM-PBSA) binding free energies suggest higher binding affinity for the HIV-1 PR-4UY interaction than HIV-1 PR-DRV interaction. We predict that the p20 and p51 mutant variants cause drug resistance against DRV while 4UY is more potent against HIV-1 PR. The present study sheds light on the dynamics of WT HIV-1 PR and mutated variants, and its inhibition by DRV and 4UY, providing useful information to the design of more potent and effective HIV-1 PR inhibitors.

Keywords: HIV-1 PR, DRV, 4UY, molecular dynamics simulation, binding free energy, principal component analysis.

Theoretical Comparative Study of Oxygen Adsorption on Neutral and Anionic Ag_n and Au_n Clusters (n = 2 − 25)

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Using density functional theory (DFT), we have performed a theoretical comparative study of oxygen adsorption on neutral and anionic Ag_n and Au_n clusters in a large size range of $n = 2 - 25$. Ionization potentials (IPs) and electron affinities (EAs) of the pure clusters and the $M_n^q - O_2$ binding energies $E_{bind}(M_n^q - O_2)$ in the $(M_nO_2)^q$ complexes (M = Ag, Au; q = 0, −1) were determined. Three density functionals, BP86, revPBE, and B3LYP were used in the calculations, among which the BP86 functional gives the best results for IPs and EAs, while B3LYP gives the best results for $E_{bind}(M_n^q - O_2)$. A number of differences between the silver and gold clusters and their reactivities toward O_2 adsorption are accounted for by the calculations. One interesting result is that the calculated $Au_n^- - O_2$ binding energies are in good, quantitative agreement with the measured relative reactivities of the Au_n^- cluster anions toward O_2 adsorption.

Is a triplet state species the origin of thermochromic behavior in a new class of phosphonium-based ionic liquids?

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Tetraphenylphosphonium bis(trifluoromethylsulfonyl)imide ([PPh$_4$][NTf$_2$]) is a colorless, low-T$_m$ salt of high thermal stability. Cation variants in which a carbazole, or similar moiety, replaces one of the phenyl groups ([PPh$_3$X][NTf$_2$]) are also colorless and generally retain the thermal stability of the parent, but surprisingly exhibit thermochromicity above T$_m$. The attained color persists after cooling and after the salt is dissolved in polar aprotic solvents; the color is lost upon introduction to polar protic solvents. Pairings with anions other than NTf$_2$ (or the similar bis(pentafluoroethylsulfonyl)imide: BETI) yield salts that are not thermochromic. Here, B3LYP/6-31G(d) optimizations and single-point TD/CAM-B3LYP/6-31G(d) excitation energies for the ground state and lowest triplet state of several PPh$_3$X cation variants are carried out to investigate the origin of this behavior. The results are consistent with thermal generation of a persistent, colored species on the triplet energy surface.

Applications of Halogen Bonding to Supramolecular Chemistry, Phosphorescence Materials and Catalysis

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Halogen Bonding (XB) has become one of the most studied non-covalent interactions in the past two decades, owing to its wide range of applications in materials and biological and catalysis applications. Due to its bond strength and directionality, halogen bonds have great potential as *supramolecular synthons* in crystal engineering and rational catalyst and drug design. In this presentation, we will report our application studies on XB to supramolecular chemistry, phosphorescence materials and catalysis. Aromatic systems are potential halogen bond acceptors in supramolecular assemblies. Our updated statistical analysis of CSD survey of halogen bond contacts and *ab initio* studies involving several polycyclic aromatic hydrocarbons and *N*-heteroaromatic compounds revealed that XB generally forms at the rim of a phenyl ring with distinct site specificity. We envisage that the predicted XB site maps will be useful for materials and drug design involving this class of non-covalent interactions [1-2]. In recent years, several groups have reported aromatic and heteroaromatic XB acceptors, such as phenanthrene, naphthalene and carbazole, exhibiting phosphorescence properties in XB assembled crystals. In an attempt to understand the application of XB on phosphorescence materials, we have carried out an ab initio study to address the fundamental questions on whether XB promotes intersystem crossing between excited states. We will report the important findings on several model systems on XB-induced phosphorescence materials [3]. For catalysis application, we have examined the use of halogen-bond donors as noncovalent activators in Lewis acid catalysis. We will report our computational studies on two halogen bonding (XB) based catalysts, namely triaryl benzene and bis-bipyridinium with multiple **iodine-containing** groups, and their applications to Diels-Alder reaction, Claisen rearrangement, cope-type hydroamination and [3+2] cycloadditions [4].

binding sites of aromatic XB acceptors
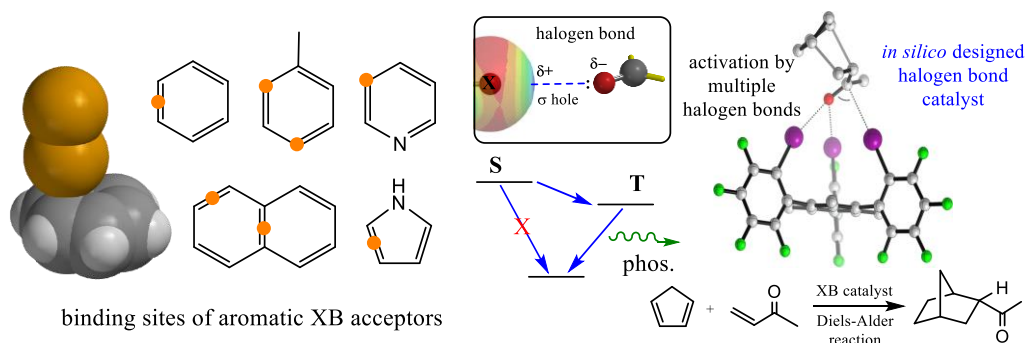
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Electrostatic Catalysis Induced by Luciferases in the Decomposition of the Firefly Dioxetanone and its Analogs

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The variations of the barrier heights in the decomposition of the firefly dioxetanone and its analogs with the electrostatic field produced by the active site amino acid residues in the firefly luciferase are examined by a DFT study for the high energy intermediates of the three luciferins. The positive electric field along the long-axis direction of the luciferins lowers the activation energy and acts as an electrostatic catalyst in the thermolysis process. The calculated barrier heights for the firefly dioxetanone and its analogs surrounded by the firefly *Photinus pyralis* luciferase show that the energy barrier of the firefly dioxetanone is lowered by the luciferase, but is raised for the other analog. Thus the thermolysis rate is enhanced for the natural D-luciferin and reduced for the other by the firefly luciferase, which elucidates why the luciferase acts as a catalyst for the natural D-luciferin but makes some luciferins emit weaker light signals.

Dynamics study of biomass pyrolysis with neural network potential

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The present knowledge of biomass pyrolysis chemistry comes from extensive contributions by early researchers working in combustion and fireproofing applications using carbohydrates and woody biomass. More than 50% of biomass comprises cellulose. That is why the main products of biomass pyrolysis are diverse cellulose intermediates and their molecular complexes. Although cellulose pyrolysis has been under the extensive studies for more than six decades, the molecular level processes underlying the pyrolysis are still under debates mainly because of the strongly differing assumption invoked by the various computational models in different periods of time.

One of the grand challenges in modern theoretical chemistry is designing and implementing approximations that expedite *ab initio* methods without loss of accuracy. In present study, we demonstrate how a deep neural network trained on quantum mechanical DFT calculations can describe the nascent decomposition processes in cellulose fast pyrolysis. We use ANAKIN-ME (Accurate NeurAl networK engINe for Molecular Energies) or ANI for short. ANI is a new method designed with the intent of developing transferable neural network potentials that utilize a highly-modified version of the Behler and Parrinello symmetry functions to build single-atom atomic environment vectors as a molecular representation.

We used a simulation cell comprised of two-unit cells of cellulose Iβ periodically repeated in three dimensions to mimic the solid cellulose. It is worth to note, that the experimental pyrolysis temperature ranges from 400–700 C with millisecond reaction time scales. In order to explore the mechanism of fast pyrolysis reactions of cellulose (where multiple products are formed from the decomposition of a single molecule in a large number of parallel reactions) without a priori knowledge of any of the pathways or use of biased reaction coordinates, the simulations were performed at higher temperatures (800–1100 C). Running simulations at these temperatures accelerates the reactions from the millisecond to the picosecond scale. Given the small simulation size, it is not possible to obtain the entire range of products observed experimentally. Hence, in an attempt to explore multiple pathways leading to multiple products (from a single starting reactant), simulations were conducted at different temperatures. Dynamics study yielded a variety of chemical reactions such as *depolymerization, fragmentation, ring opening*, and *ring contraction*. These reactions yielded precursors to levoglucosan (LGA) - the major product of pyrolysis - and also to minor products such as 5-hydroxy-methylfurfural (HMF) and formic acid. At T > 600 °C, we found that depolymerization via ring contraction of the glucopyranose ring to the glucofuranose ring occurs with the lowest free-energy barrier (20 kcal/mol). We suggest that this process is key for formation of liquid intermediate cellulose, observed experimentally. At > 800 °C, we found that a precursor to LGA (pre-LGA) forms with a free-energy barrier of 36 kcal/mol via an

intermediate/transition state stabilized by hydrogen bonding. We found that free-energy barriers at 900 °C are in the order pre-LGA < pre-HMF < formic acid, explaining why LGA is the kinetically favored product of fast cellulose pyrolysis.

AIMNet: atom-in-molecule neural network multimodal potential

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Computational modeling of chemical and biological systems at atomic resolution has become a crucial tool in the chemist's toolset. The use of computer simulations has always required a balance between cost and accuracy: Quantum-mechanical (QM) methods provide the highest accuracy for simulating molecules but are computationally expensive and have difficulty scaling to large systems, while empirical interatomic potentials (classical force fields) are cheap and scalable, but lack transferability to new systems and are hard to systematically improve. Neural network potentials (NNP) represent a data-driven approach to construct force-field like molecular potentials. The main idea behind this type of potentials is utilization of deep neural networks to approximate very complex potential energy surfaces. Such approach can provide much better accuracy compared to classical force fields, while it requires about the same computational resources as force field methods, and millions of times less than ab initio QM methods. Even more important, with careful construction of the model and proper training dataset, the NNP demonstrate good extensibility and transferability, which make excellent methods for application towards real-world problems.

We present the AIMNet (Atom-in-Molecule Network) a chemically inspired, modular deep neural network molecular potential We use multimodal and multi-task learning to obtain information-rich representation of an atom in a molecule. The resulting model shows the state-of-the-art accuracy, comparable to orders of magnitude more expensive DFT methods on several benchmark datasets. It can simultaneously predict energies, atomic charges, and volumes without compromising accuracy and increase of computational cost. We also show how the multimodal information about the atom state could be used to efficiently learn new properties, like solvation free energies, with much less training data.